



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:00 PM UTC

PDB ID : 4A3M / pdb_00004a3m
Title : RNA Polymerase II initial transcribing complex with a 4nt DNA-RNA hybrid and soaked with AMPCPP
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

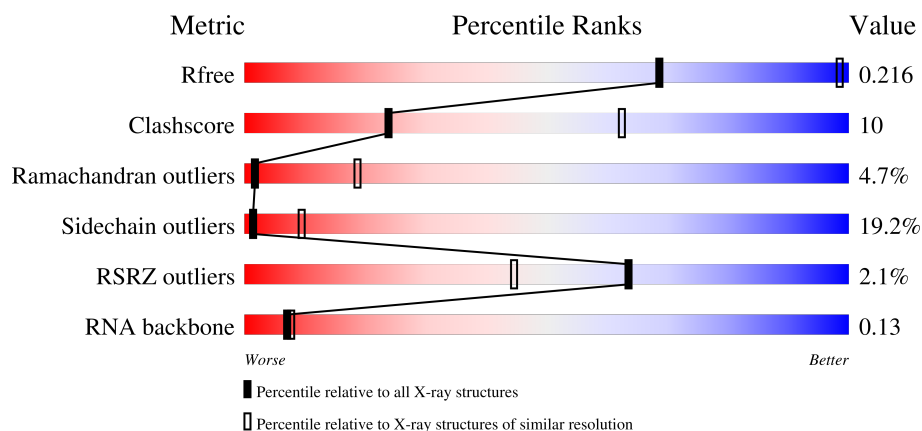
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1732	 2% 47% 27% 7% 18%
2	B	1224	 2% 54% 29% 8% 9%
3	C	318	 44% 30% 9% 16%
4	D	221	 3% 48% 26% 6% 19%

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Mol	Chain	Length	Quality of chain
5	E	215	% 66% 28% 5%
6	F	155	% 34% 16% 46%
7	G	171	61% 28% 10%
8	H	146	6% 51% 31% 6% 9%
9	I	122	3% 64% 28% 5%
10	J	70	% 51% 26% 11% 7%
11	K	120	% 53% 35% 8%
12	L	70	7% 27% 27% 9% 34%
13	N	14	14% 57% 7% 36%
14	P	4	25% 75%
15	T	26	4% 31% 31% 35%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			183	89	34	52	8			

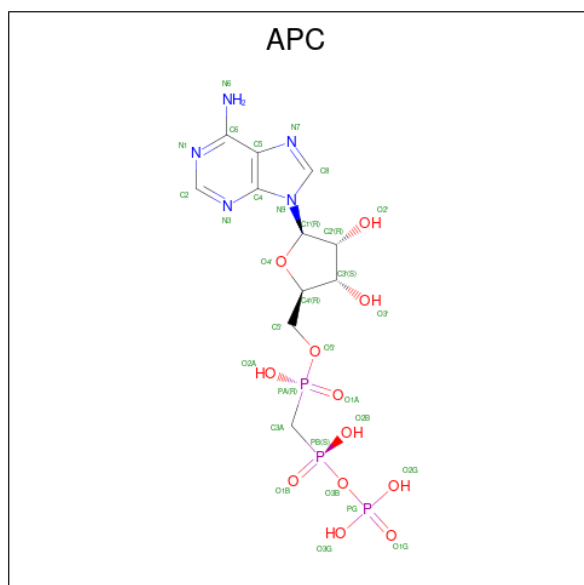
- Molecule 14 is a RNA chain called 5'-R(*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	17	Total	Br	C	N	O	P	0	0
			345	1	165	56	106	17		

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	B	1	Total 1	Zn 1	0	0
17	C	1	Total 1	Zn 1	0	0
17	I	2	Total 2	Zn 2	0	0
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

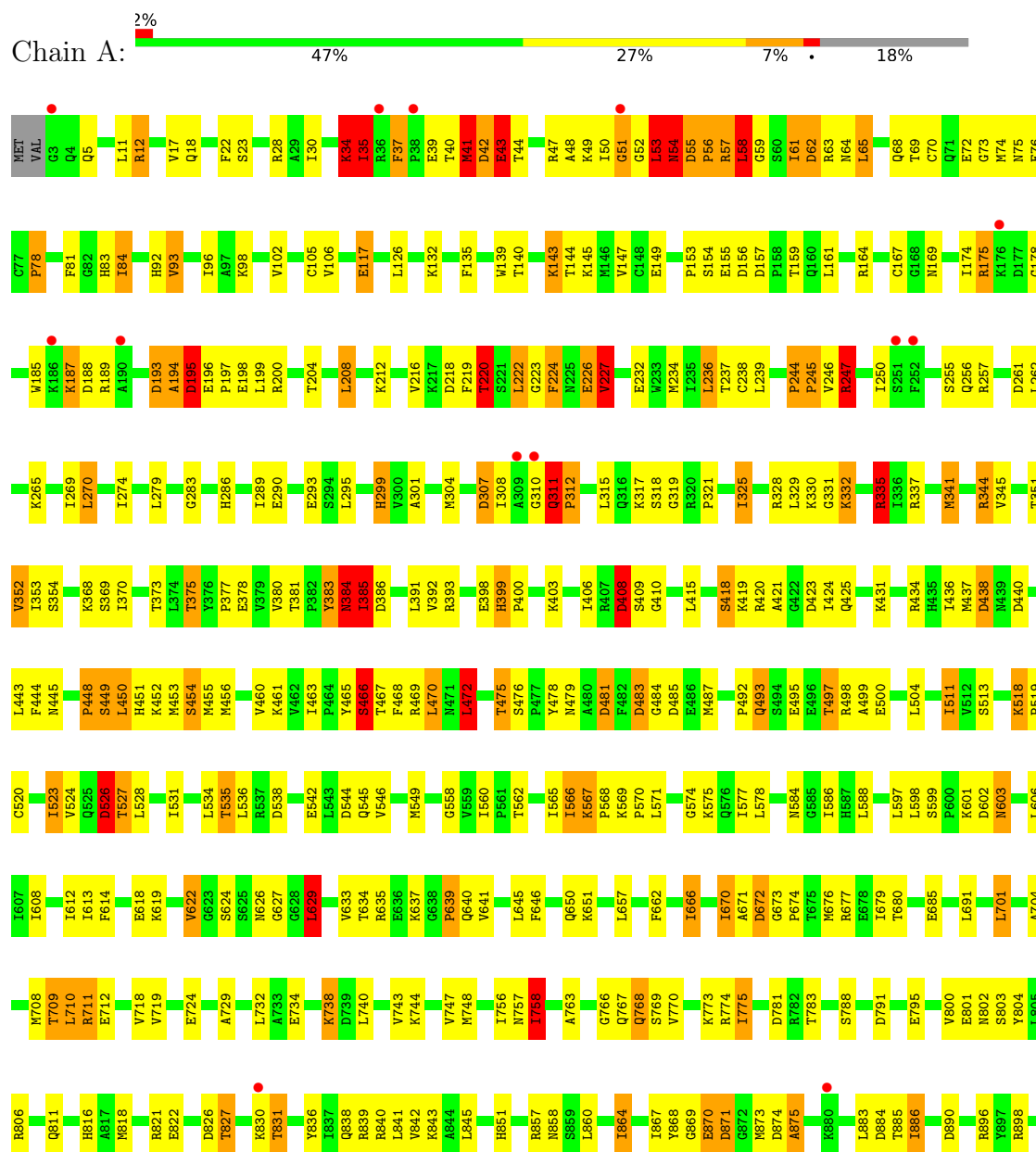
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

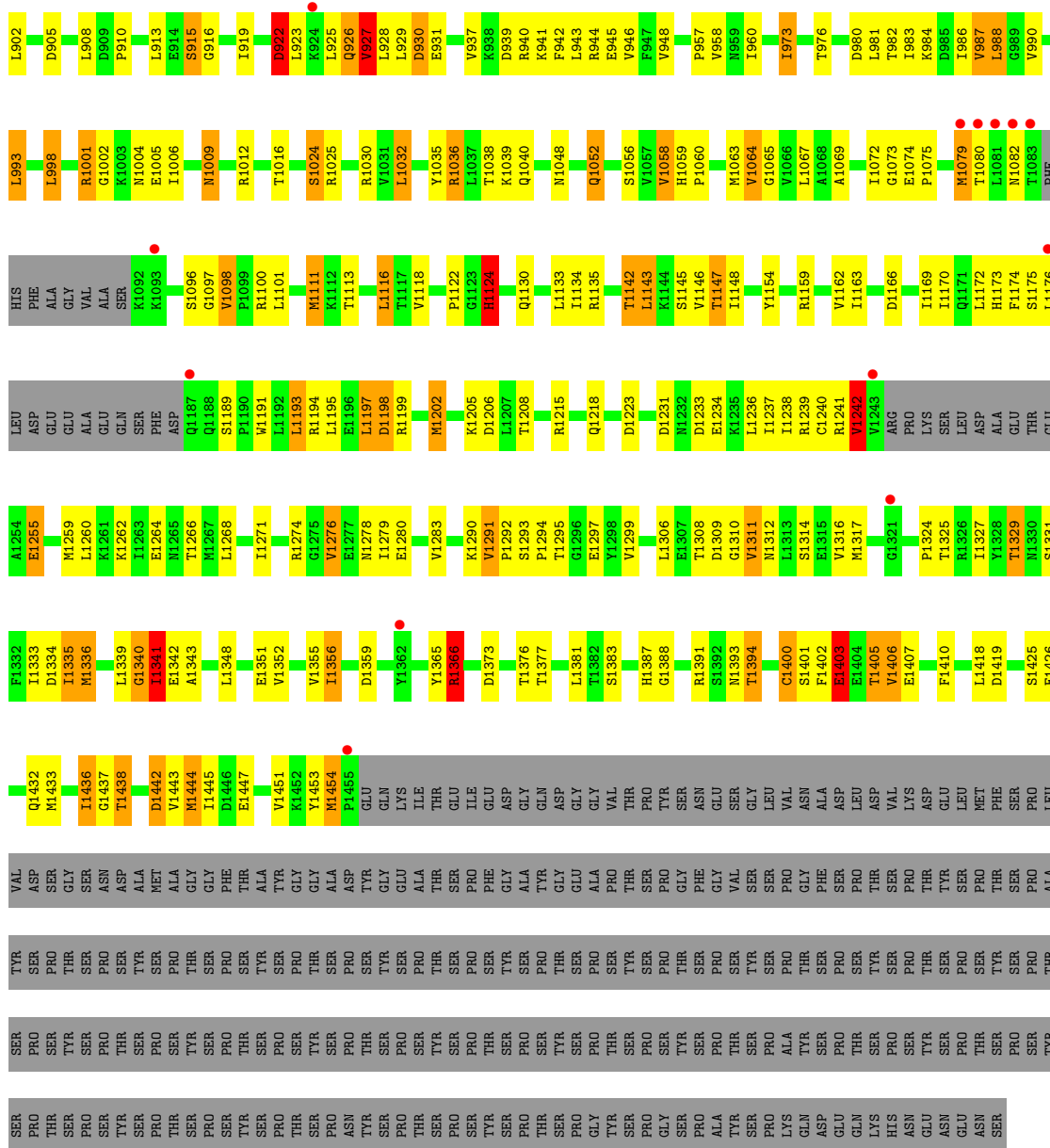
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

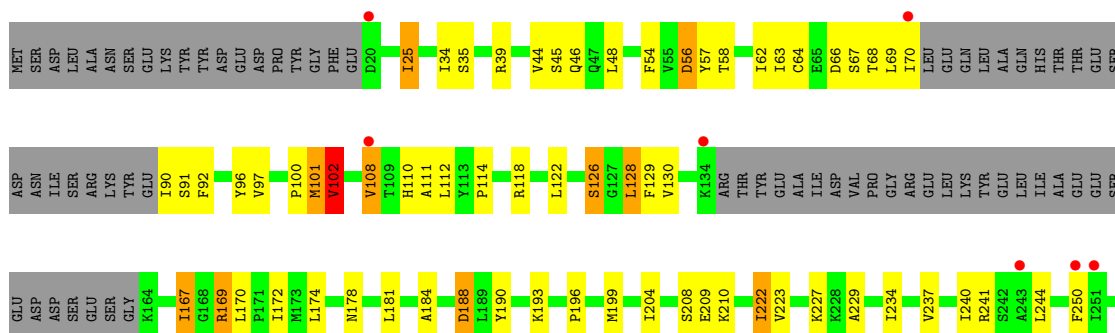
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

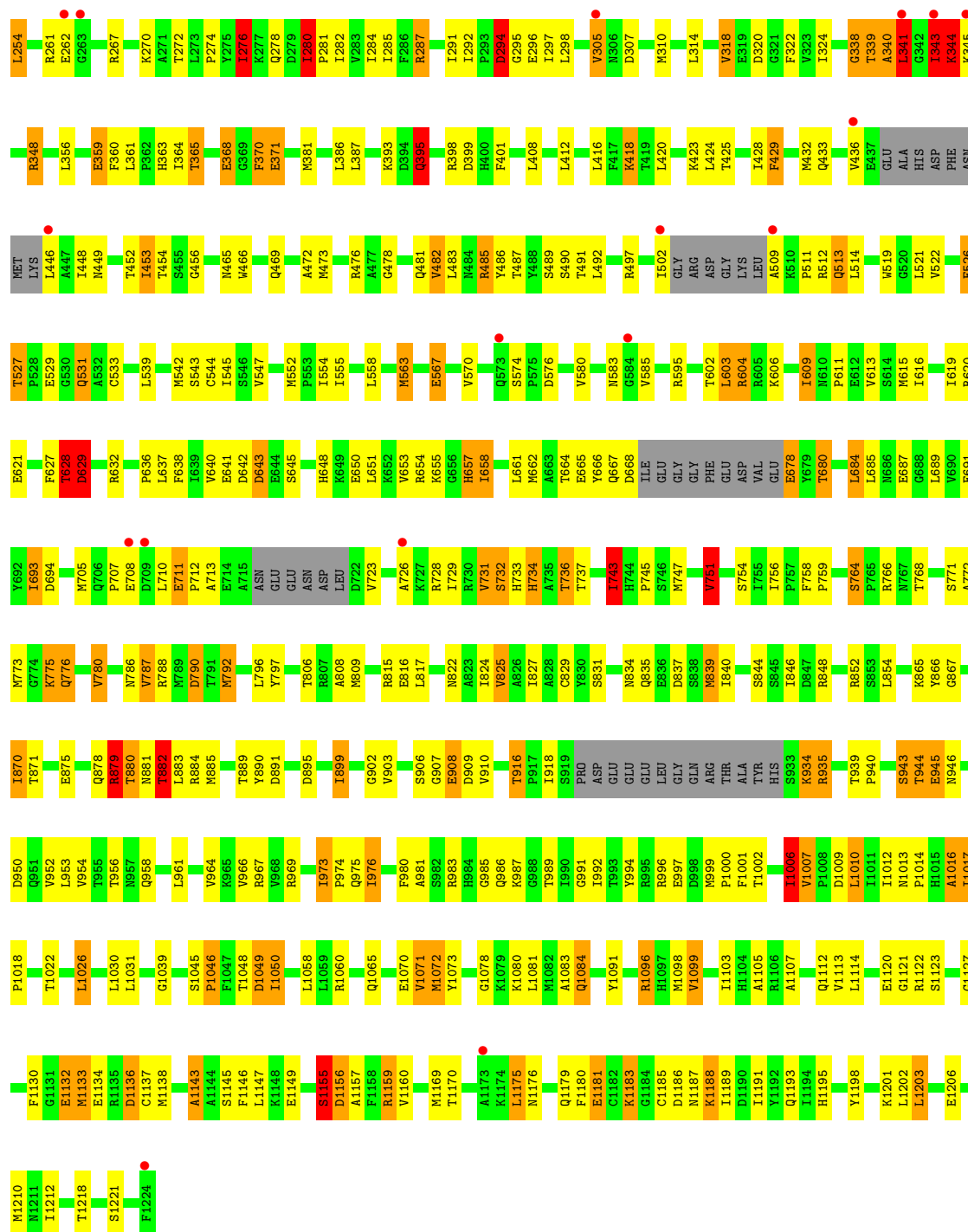
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

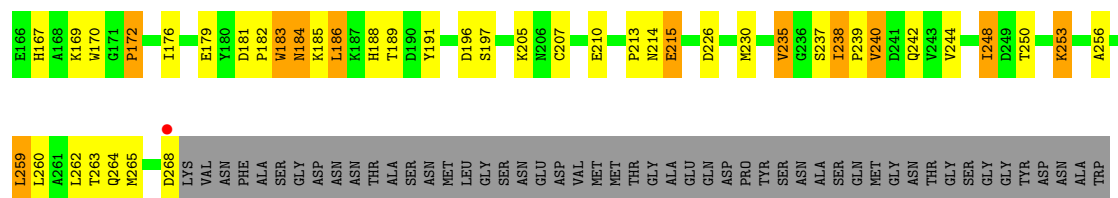




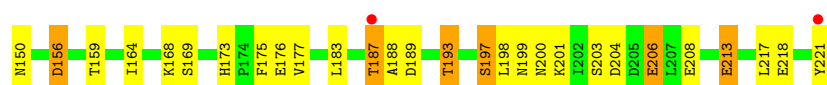
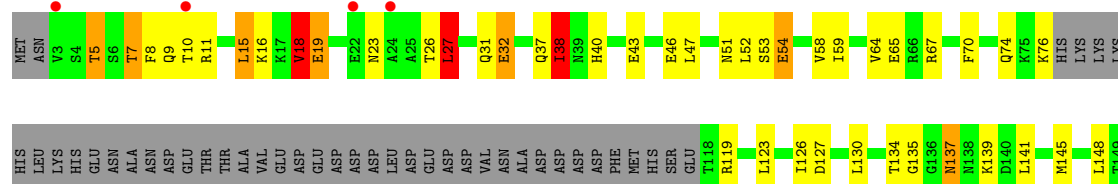
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



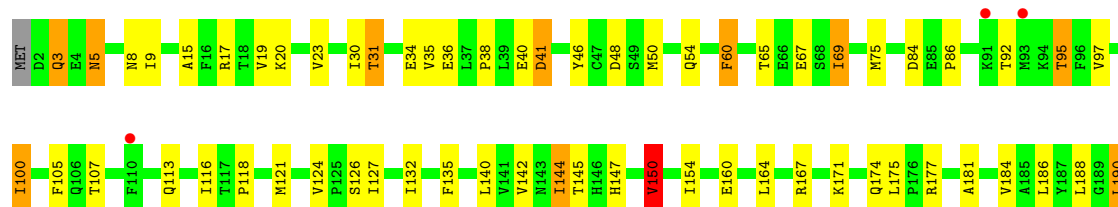




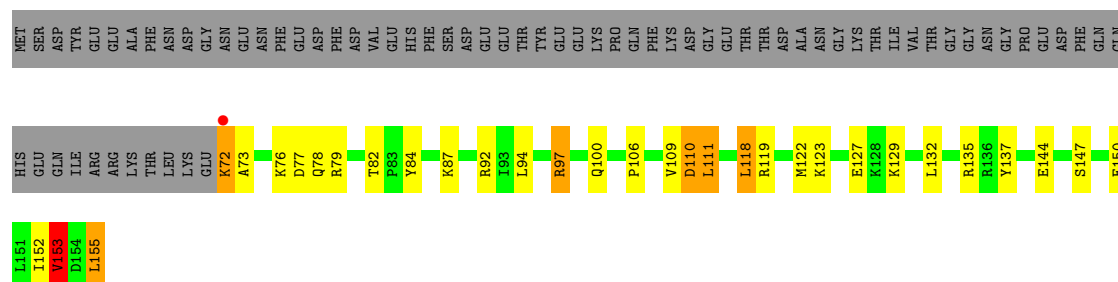
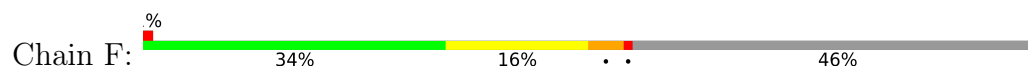
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

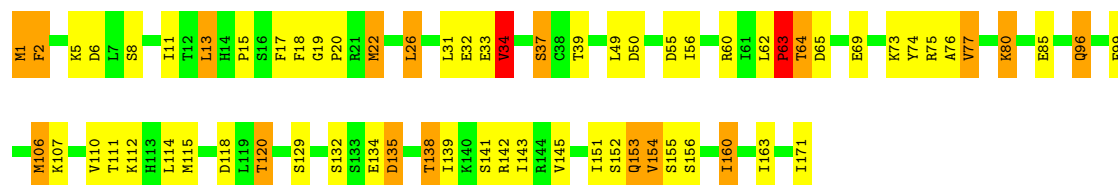


• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

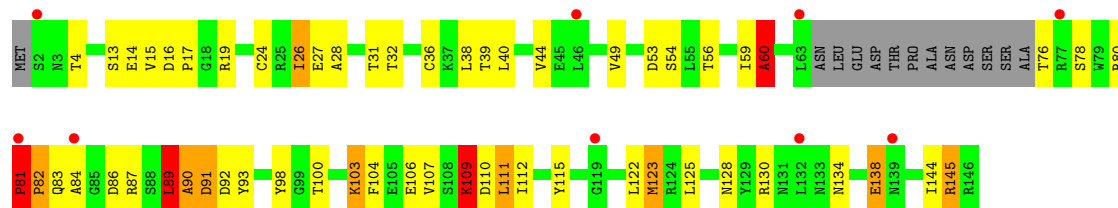


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

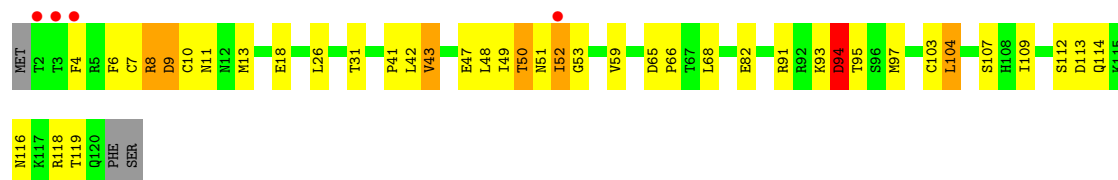




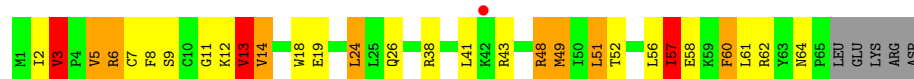
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



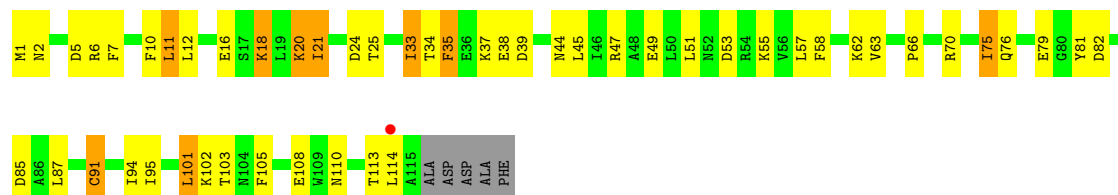
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



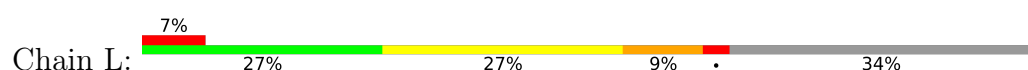
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5

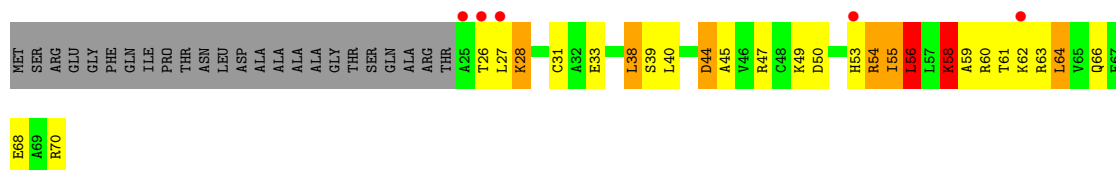


- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

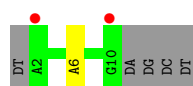


- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

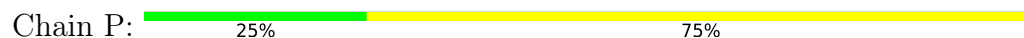




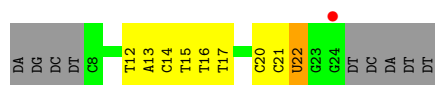
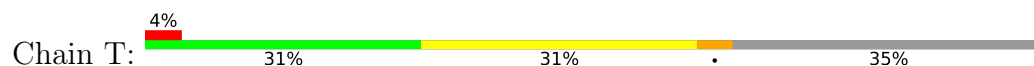
- Molecule 13: 5'-D(*AP*AP*GP*TP*AP*CP*TP)-3'



- Molecule 14: 5'-R(*AP*GP*GP*A)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP* TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.27Å 392.99Å 282.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.65 – 3.90 58.65 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.65-3.90) 99.2 (58.65-3.90)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.154 , 0.190 0.186 , 0.216	Depositor DCC
R_{free} test set	2247 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	131.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 145.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.057 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31868	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, APC, MG, BRU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	11/11397 (0.1%)	1.62	164/15415 (1.1%)
2	B	0.89	2/9029 (0.0%)	1.54	128/12171 (1.1%)
3	C	0.86	1/2133 (0.0%)	1.52	31/2891 (1.1%)
4	D	0.89	0/1444	1.62	17/1935 (0.9%)
5	E	0.79	0/1788	1.46	18/2406 (0.7%)
6	F	0.95	0/691	1.47	8/933 (0.9%)
7	G	0.86	1/1368 (0.1%)	1.43	13/1844 (0.7%)
8	H	0.91	0/1086	1.55	21/1470 (1.4%)
9	I	0.80	0/989	1.40	14/1331 (1.1%)
10	J	0.93	1/541 (0.2%)	1.54	4/727 (0.6%)
11	K	0.82	0/938	1.55	17/1267 (1.3%)
12	L	0.87	0/365	1.50	5/485 (1.0%)
13	N	0.57	0/205	0.74	0/315
14	P	0.55	0/101	0.71	0/156
15	T	0.59	0/361	0.69	0/552
All	All	0.88	16/32436 (0.0%)	1.54	440/43898 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	CA-C	-9.57	1.46	1.53
1	A	57	ARG	CA-C	6.60	1.61	1.52
10	J	49	MET	SD-CE	-6.41	1.63	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	6.24	1.42	1.33
1	A	54	ASN	CA-C	5.95	1.60	1.52
1	A	1454	MET	CA-C	5.61	1.59	1.52
2	B	1180	PHE	CA-C	-5.57	1.48	1.52
2	B	944	THR	CA-CB	5.37	1.61	1.53
1	A	256	GLN	CA-C	5.35	1.58	1.53
7	G	1	MET	C-N	5.32	1.41	1.33
1	A	867	ILE	CG1-CD1	5.31	1.72	1.51
3	C	181	ASP	CA-CB	5.27	1.56	1.52
1	A	56	PRO	CA-C	5.16	1.59	1.52
1	A	1336	MET	SD-CE	5.12	1.92	1.79
1	A	53	LEU	N-CA	5.07	1.51	1.45
1	A	247	ARG	CA-C	5.01	1.58	1.53

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	MET	CA-C-N	10.92	129.08	121.65
1	A	341	MET	C-N-CA	10.92	129.08	121.65
4	D	26	THR	N-CA-C	-9.69	98.48	110.88
8	H	92	ASP	N-CA-C	-9.56	98.39	111.87
1	A	56	PRO	CA-C-N	9.20	139.11	121.54
1	A	56	PRO	C-N-CA	9.20	139.11	121.54
1	A	54	ASN	CA-C-N	9.10	132.66	122.83
1	A	54	ASN	C-N-CA	9.10	132.66	122.83
1	A	483	ASP	CA-CB-CG	8.75	121.35	112.60
10	J	5	VAL	N-CA-C	-8.53	97.63	108.89
5	E	60	PHE	CA-CB-CG	8.47	122.27	113.80
2	B	1136	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	864	ILE	N-CA-C	-8.42	103.62	111.45
11	K	2	ASN	CA-C-N	8.15	131.73	120.65
11	K	2	ASN	C-N-CA	8.15	131.73	120.65
1	A	34	LYS	CA-C-N	8.09	136.27	121.70
1	A	34	LYS	C-N-CA	8.09	136.27	121.70
5	E	150	VAL	N-CA-C	8.09	115.93	107.76
2	B	943	SER	CA-C-N	8.07	130.94	120.44
2	B	943	SER	C-N-CA	8.07	130.94	120.44
1	A	526	ASP	CA-CB-CG	7.84	120.44	112.60
2	B	694	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	886	ILE	N-CA-C	7.62	117.70	110.30
1	A	194	ALA	CA-C-N	7.62	135.42	121.70
1	A	194	ALA	C-N-CA	7.62	135.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	44	ASN	CA-C-N	7.58	130.30	120.44
11	K	44	ASN	C-N-CA	7.58	130.30	120.44
2	B	296	GLU	N-CA-C	-7.56	101.94	112.45
1	A	218	ASP	CA-CB-CG	7.49	120.09	112.60
2	B	338	GLY	CA-C-N	7.48	135.16	121.70
2	B	338	GLY	C-N-CA	7.48	135.16	121.70
2	B	1071	VAL	N-CA-CB	7.48	119.53	111.00
1	A	244	PRO	N-CA-C	7.47	119.81	110.70
1	A	724	GLU	N-CA-C	-7.29	102.94	111.03
1	A	42	ASP	CA-CB-CG	7.23	119.83	112.60
2	B	890	TYR	CA-C-N	7.22	130.93	120.38
2	B	890	TYR	C-N-CA	7.22	130.93	120.38
2	B	881	ASN	N-CA-C	7.22	121.39	112.58
1	A	511	ILE	N-CA-CB	7.15	118.45	110.51
1	A	1407	GLU	CA-C-N	7.13	129.69	120.56
1	A	1407	GLU	C-N-CA	7.13	129.69	120.56
8	H	81	PRO	N-CA-C	7.11	119.38	110.70
2	B	1016	ALA	CA-C-N	7.11	127.25	120.43
2	B	1016	ALA	C-N-CA	7.11	127.25	120.43
1	A	424	ILE	CA-C-N	-7.08	113.64	122.84
1	A	424	ILE	C-N-CA	-7.08	113.64	122.84
1	A	75	ASN	N-CA-C	-7.03	100.08	110.48
1	A	35	ILE	N-CA-CB	7.02	123.43	111.50
3	C	40	GLU	N-CA-C	7.00	121.27	112.87
8	H	138	GLU	N-CA-C	-6.98	103.76	111.36
1	A	219	PHE	CA-CB-CG	6.95	120.75	113.80
2	B	736	THR	N-CA-C	-6.95	103.98	113.30
1	A	874	ASP	CA-CB-CG	6.88	119.48	112.60
11	K	63	VAL	N-CA-CB	6.86	119.47	111.66
4	D	188	ALA	N-CA-C	-6.85	104.03	112.38
1	A	445	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	1202	MET	CA-C-N	6.82	129.73	120.38
1	A	1202	MET	C-N-CA	6.82	129.73	120.38
1	A	1097	GLY	CA-C-N	6.75	126.92	120.43
1	A	1097	GLY	C-N-CA	6.75	126.92	120.43
3	C	56	THR	N-CA-C	6.75	120.37	110.59
1	A	875	ALA	N-CA-C	6.74	119.64	111.82
9	I	93	LYS	CA-C-N	6.74	130.93	120.82
9	I	93	LYS	C-N-CA	6.74	130.93	120.82
7	G	63	PRO	N-CA-C	6.74	126.35	112.47
8	H	110	ASP	N-CA-C	-6.74	104.62	114.39
6	F	87	LYS	CA-C-N	6.71	129.57	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	87	LYS	C-N-CA	6.71	129.57	120.44
3	C	56	THR	CA-C-N	6.70	131.77	120.64
3	C	56	THR	C-N-CA	6.70	131.77	120.64
2	B	1006	ILE	N-CA-CB	6.69	117.82	110.53
1	A	627	GLY	CA-C-N	6.66	126.42	120.10
1	A	627	GLY	C-N-CA	6.66	126.42	120.10
3	C	205	LYS	N-CA-C	-6.64	103.97	111.07
4	D	31	GLN	N-CA-C	-6.63	104.94	113.16
6	F	132	LEU	N-CA-C	6.61	120.26	110.48
2	B	1022	THR	CB-CA-C	6.59	121.82	112.07
7	G	34	VAL	N-CA-C	6.59	117.34	110.62
3	C	136	ASP	CA-CB-CG	6.57	119.17	112.60
2	B	1155	SER	CA-C-N	6.56	134.06	121.54
2	B	1155	SER	C-N-CA	6.56	134.06	121.54
2	B	1132	GLU	CA-C-N	6.53	129.02	120.28
2	B	1132	GLU	C-N-CA	6.53	129.02	120.28
3	C	230	MET	N-CA-C	6.52	119.08	109.24
1	A	384	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	149	GLU	N-CA-C	6.51	119.31	108.96
2	B	964	VAL	N-CA-C	6.51	117.67	108.17
1	A	47	ARG	CA-C-N	6.50	133.95	121.54
1	A	47	ARG	C-N-CA	6.50	133.95	121.54
1	A	385	ILE	CA-C-N	6.49	129.30	120.54
1	A	385	ILE	C-N-CA	6.49	129.30	120.54
3	C	145	CYS	N-CA-C	6.48	116.62	108.45
4	D	38	ILE	N-CA-C	6.46	116.78	108.12
3	C	45	ALA	CA-C-N	6.46	129.22	120.63
3	C	45	ALA	C-N-CA	6.46	129.22	120.63
3	C	213	PRO	N-CA-C	6.45	121.96	114.03
1	A	535	THR	N-CA-C	6.42	120.35	111.55
11	K	39	ASP	CA-C-N	6.39	129.71	120.38
11	K	39	ASP	C-N-CA	6.39	129.71	120.38
4	D	169	SER	CA-C-N	6.38	129.69	120.38
4	D	169	SER	C-N-CA	6.38	129.69	120.38
1	A	223	GLY	CA-C-N	6.36	133.69	121.54
1	A	223	GLY	C-N-CA	6.36	133.69	121.54
1	A	68	GLN	CA-C-N	6.35	133.67	121.54
1	A	68	GLN	C-N-CA	6.35	133.67	121.54
1	A	1032	LEU	N-CA-C	6.33	119.13	111.40
1	A	858	ASN	CA-C-N	6.33	129.05	120.38
1	A	858	ASN	C-N-CA	6.33	129.05	120.38
1	A	34	LYS	N-CA-C	-6.32	97.98	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	1419	ASP	N-CA-C	6.29	118.99	108.73
2	B	45	SER	CA-C-N	6.28	129.51	120.79
2	B	45	SER	C-N-CA	6.28	129.51	120.79
2	B	307	ASP	CA-C-N	6.26	129.53	120.38
2	B	307	ASP	C-N-CA	6.26	129.53	120.38
1	A	307	ASP	CA-C-N	6.26	131.18	121.85
1	A	307	ASP	C-N-CA	6.26	131.18	121.85
2	B	188	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	811	GLN	N-CA-C	-6.24	104.11	111.03
2	B	66	ASP	CA-C-N	6.21	130.13	120.82
2	B	66	ASP	C-N-CA	6.21	130.13	120.82
9	I	9	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	319	GLY	CA-C-N	6.16	129.03	120.65
1	A	319	GLY	C-N-CA	6.16	129.03	120.65
1	A	1406	VAL	CA-C-N	6.15	128.52	120.28
1	A	1406	VAL	C-N-CA	6.15	128.52	120.28
2	B	1179	GLN	CA-C-N	-6.14	114.28	121.64
2	B	1179	GLN	C-N-CA	-6.14	114.28	121.64
1	A	622	VAL	N-CA-CB	-6.13	104.13	112.28
3	C	112	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	998	LEU	N-CA-C	6.12	119.49	109.76
1	A	677	ARG	CA-C-N	6.09	128.45	120.28
1	A	677	ARG	C-N-CA	6.09	128.45	120.28
2	B	628	THR	CA-C-N	6.09	133.17	121.54
2	B	628	THR	C-N-CA	6.09	133.17	121.54
1	A	558	GLY	CA-C-N	6.08	129.97	122.37
1	A	558	GLY	C-N-CA	6.08	129.97	122.37
1	A	1231	ASP	CA-C-N	6.05	128.39	120.28
1	A	1231	ASP	C-N-CA	6.05	128.39	120.28
4	D	54	GLU	N-CA-C	-6.05	104.68	111.28
8	H	36	CYS	N-CA-C	6.05	119.51	109.46
1	A	472	LEU	N-CA-C	6.05	118.84	111.82
5	E	95	THR	CA-C-N	6.04	128.38	120.28
5	E	95	THR	C-N-CA	6.04	128.38	120.28
1	A	72	GLU	N-CA-C	6.01	118.36	111.02
2	B	958	GLN	CA-C-N	6.01	128.83	120.29
2	B	958	GLN	C-N-CA	6.01	128.83	120.29
1	A	1419	ASP	CA-C-N	6.00	128.64	120.54
1	A	1419	ASP	C-N-CA	6.00	128.64	120.54
12	L	49	LYS	CA-C-N	6.00	133.00	121.54
12	L	49	LYS	C-N-CA	6.00	133.00	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ASP	CA-CB-CG	5.99	118.59	112.60
3	C	26	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	710	LEU	N-CA-C	-5.99	104.76	111.28
2	B	1175	LEU	N-CA-C	5.98	120.31	113.19
2	B	1122	ARG	CA-C-N	5.98	128.61	120.54
2	B	1122	ARG	C-N-CA	5.98	128.61	120.54
2	B	1130	PHE	CA-C-N	5.97	126.95	120.44
2	B	1130	PHE	C-N-CA	5.97	126.95	120.44
10	J	9	SER	N-CA-C	5.97	117.46	111.07
5	E	5	ASN	N-CA-C	-5.97	105.08	112.90
3	C	183	TRP	N-CA-C	-5.97	98.80	108.41
1	A	408	ASP	CA-CB-CG	5.95	118.55	112.60
7	G	64	THR	CB-CA-C	5.93	120.20	110.17
1	A	1079	MET	N-CA-C	-5.93	106.20	113.50
7	G	50	ASP	CA-CB-CG	5.93	118.53	112.60
3	C	238	ILE	CB-CA-C	5.92	115.14	109.33
1	A	55	ASP	N-CA-CB	5.91	119.96	111.51
8	H	53	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	399	HIS	CA-CB-CG	-5.85	107.95	113.80
2	B	339	THR	CA-C-N	5.84	132.70	121.54
2	B	339	THR	C-N-CA	5.84	132.70	121.54
8	H	90	ALA	CA-C-N	5.84	130.43	122.84
8	H	90	ALA	C-N-CA	5.84	130.43	122.84
2	B	1078	GLY	CA-C-N	5.83	129.64	121.02
2	B	1078	GLY	C-N-CA	5.83	129.64	121.02
3	C	196	ASP	CA-C-N	5.83	128.40	120.54
3	C	196	ASP	C-N-CA	5.83	128.40	120.54
2	B	879	ARG	CA-C-N	5.82	132.65	121.54
2	B	879	ARG	C-N-CA	5.82	132.65	121.54
1	A	193	ASP	CA-C-N	5.82	132.17	121.70
1	A	193	ASP	C-N-CA	5.82	132.17	121.70
1	A	226	GLU	N-CA-C	5.81	119.47	112.38
7	G	33	GLU	CA-C-N	5.81	128.42	120.46
7	G	33	GLU	C-N-CA	5.81	128.42	120.46
8	H	110	ASP	CA-CB-CG	5.80	118.40	112.60
2	B	343	ILE	CA-C-N	5.80	132.61	121.54
2	B	343	ILE	C-N-CA	5.80	132.61	121.54
3	C	39	ALA	N-CA-C	5.80	120.02	111.04
4	D	156	ASP	N-CA-C	5.79	118.65	109.50
1	A	399	HIS	N-CA-CB	5.78	120.66	110.37
2	B	684	LEU	CA-C-N	5.78	128.34	120.54
2	B	684	LEU	C-N-CA	5.78	128.34	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	53	ASP	CA-CB-CG	5.77	118.37	112.60
2	B	768	THR	CA-C-N	5.76	130.34	120.71
2	B	768	THR	C-N-CA	5.76	130.34	120.71
2	B	222	ILE	CB-CA-C	5.76	118.19	110.42
1	A	1340	GLY	CA-C-N	5.76	132.33	121.97
1	A	1340	GLY	C-N-CA	5.76	132.33	121.97
2	B	254	LEU	N-CA-C	5.75	117.90	108.52
4	D	26	THR	CA-C-N	5.74	132.51	121.54
4	D	26	THR	C-N-CA	5.74	132.51	121.54
9	I	53	GLY	CA-C-N	5.73	128.21	120.65
9	I	53	GLY	C-N-CA	5.73	128.21	120.65
2	B	939	THR	CB-CA-C	5.72	115.83	110.17
1	A	757	ASN	CA-C-N	5.72	127.98	120.60
1	A	757	ASN	C-N-CA	5.72	127.98	120.60
1	A	781	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	766	GLY	N-CA-C	5.71	118.20	111.63
1	A	841	LEU	CA-C-N	5.70	128.57	120.53
1	A	841	LEU	C-N-CA	5.70	128.57	120.53
1	A	1001	ARG	N-CA-C	5.69	120.36	112.45
1	A	495	GLU	N-CA-C	-5.68	106.19	113.01
2	B	837	ASP	CA-CB-CG	5.68	118.28	112.60
2	B	687	GLU	N-CA-C	-5.68	106.39	113.38
1	A	227	VAL	N-CA-C	5.67	116.50	111.90
2	B	56	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	988	LEU	N-CA-C	5.67	117.54	111.36
1	A	1325	THR	N-CA-C	-5.67	106.24	114.12
8	H	86	ASP	CA-C-N	5.66	129.14	120.82
8	H	86	ASP	C-N-CA	5.66	129.14	120.82
12	L	58	LYS	N-CA-C	5.66	121.21	113.97
1	A	5	GLN	N-CA-C	5.65	118.85	110.48
6	F	153	VAL	N-CA-C	5.65	114.95	106.42
1	A	245	PRO	CA-C-N	5.65	129.02	122.35
1	A	245	PRO	C-N-CA	5.65	129.02	122.35
1	A	710	LEU	CA-C-N	5.65	127.78	120.44
1	A	710	LEU	C-N-CA	5.65	127.78	120.44
2	B	555	ILE	CA-C-N	5.64	127.78	120.44
2	B	555	ILE	C-N-CA	5.64	127.78	120.44
1	A	800	VAL	CA-C-N	5.64	128.40	120.28
1	A	800	VAL	C-N-CA	5.64	128.40	120.28
2	B	478	GLY	CA-C-N	5.64	128.18	120.46
2	B	478	GLY	C-N-CA	5.64	128.18	120.46
1	A	408	ASP	N-CA-C	-5.63	105.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	825	VAL	N-CA-C	5.63	116.20	107.99
7	G	153	GLN	CA-C-N	5.62	132.08	121.97
7	G	153	GLN	C-N-CA	5.62	132.08	121.97
4	D	204	ASP	CA-C-N	5.61	127.80	120.28
4	D	204	ASP	C-N-CA	5.61	127.80	120.28
3	C	191	TYR	N-CA-C	5.60	118.36	109.96
1	A	1311	VAL	N-CA-C	5.60	116.19	108.12
11	K	75	ILE	N-CA-C	5.59	116.64	107.24
3	C	55	THR	N-CA-C	-5.59	105.77	112.59
5	E	144	ILE	N-CA-CB	5.59	116.71	110.62
2	B	68	THR	CB-CA-C	5.58	118.83	109.89
1	A	17	VAL	N-CA-CB	5.58	118.90	112.15
1	A	927	VAL	N-CA-C	-5.57	105.09	110.72
5	E	171	LYS	N-CA-C	-5.57	100.81	109.72
1	A	37	PHE	N-CA-C	5.57	118.31	109.40
2	B	276	ILE	CA-C-N	5.56	127.99	120.38
2	B	276	ILE	C-N-CA	5.56	127.99	120.38
2	B	1143	ALA	CA-C-N	5.56	128.04	120.54
2	B	1143	ALA	C-N-CA	5.56	128.04	120.54
1	A	452	LYS	N-CA-C	-5.55	105.31	111.36
9	I	91	ARG	N-CA-C	5.55	119.59	113.21
12	L	60	ARG	N-CA-C	5.54	117.45	110.24
1	A	317	LYS	CA-C-N	5.53	132.09	121.54
1	A	317	LYS	C-N-CA	5.53	132.09	121.54
2	B	628	THR	N-CA-C	-5.53	106.58	113.38
2	B	950	ASP	CA-CB-CG	5.53	118.12	112.60
2	B	102	VAL	N-CA-C	5.52	116.06	107.28
11	K	82	ASP	CA-CB-CG	5.52	118.12	112.60
12	L	62	LYS	N-CA-C	-5.52	105.42	111.82
5	E	54	GLN	CA-C-N	5.51	127.66	120.28
5	E	54	GLN	C-N-CA	5.51	127.66	120.28
11	K	113	THR	CB-CA-C	5.51	119.95	111.85
7	G	135	ASP	N-CA-C	5.50	118.23	109.81
1	A	758	ILE	CA-C-N	5.50	127.58	120.44
1	A	758	ILE	C-N-CA	5.50	127.58	120.44
1	A	1233	ASP	CA-C-N	5.49	129.06	120.82
1	A	1233	ASP	C-N-CA	5.49	129.06	120.82
1	A	224	PHE	N-CA-C	5.48	122.47	110.80
3	C	259	LEU	CA-C-N	5.48	127.88	120.65
3	C	259	LEU	C-N-CA	5.48	127.88	120.65
9	I	113	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	39	ARG	N-CA-C	-5.46	105.02	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1205	LYS	CA-C-N	5.46	131.97	121.54
1	A	1205	LYS	C-N-CA	5.46	131.97	121.54
1	A	1403	GLU	CB-CG-CD	5.46	121.88	112.60
1	A	311	GLN	N-CA-C	5.45	121.86	109.81
11	K	110	ASN	CA-C-N	5.44	127.57	120.28
11	K	110	ASN	C-N-CA	5.44	127.57	120.28
7	G	63	PRO	CA-C-N	-5.43	114.07	122.49
7	G	63	PRO	C-N-CA	-5.43	114.07	122.49
8	H	16	ASP	N-CA-C	5.42	119.04	108.85
1	A	993	LEU	N-CA-C	-5.41	105.47	111.36
1	A	495	GLU	CB-CG-CD	5.41	121.79	112.60
2	B	751	VAL	CA-C-N	5.41	127.52	120.28
2	B	751	VAL	C-N-CA	5.41	127.52	120.28
2	B	399	ASP	N-CA-C	5.40	118.98	112.93
1	A	544	ASP	CA-C-N	5.40	129.81	120.58
1	A	544	ASP	C-N-CA	5.40	129.81	120.58
2	B	1099	VAL	N-CA-CB	5.39	116.86	110.55
6	F	127	GLU	CA-C-N	5.39	130.01	122.08
6	F	127	GLU	C-N-CA	5.39	130.01	122.08
1	A	1082	ASN	CA-CB-CG	5.39	117.99	112.60
4	D	51	ASN	CA-CB-CG	5.38	117.98	112.60
8	H	109	LYS	CA-C-N	5.38	130.21	121.98
8	H	109	LYS	C-N-CA	5.38	130.21	121.98
1	A	870	GLU	CB-CG-CD	5.38	121.74	112.60
2	B	57	TYR	CA-C-N	5.38	127.75	120.38
2	B	57	TYR	C-N-CA	5.38	127.75	120.38
2	B	48	LEU	N-CA-C	5.38	116.82	111.07
2	B	280	ILE	N-CA-C	5.37	113.25	108.63
2	B	693	ILE	N-CA-C	5.37	115.51	107.51
4	D	7	THR	CA-C-N	5.37	129.69	120.72
4	D	7	THR	C-N-CA	5.37	129.69	120.72
2	B	340	ALA	CA-C-N	5.36	131.79	121.54
2	B	340	ALA	C-N-CA	5.36	131.79	121.54
2	B	650	GLU	CA-C-N	5.36	129.92	121.56
2	B	650	GLU	C-N-CA	5.36	129.92	121.56
1	A	220	THR	CB-CA-C	5.36	120.95	110.67
2	B	902	GLY	CA-C-N	5.36	131.61	121.97
2	B	902	GLY	C-N-CA	5.36	131.61	121.97
2	B	680	THR	N-CA-C	5.35	116.91	109.31
9	I	66	PRO	CA-C-N	5.35	128.19	120.38
9	I	66	PRO	C-N-CA	5.35	128.19	120.38
11	K	24	ASP	CA-C-N	5.34	127.88	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	24	ASP	C-N-CA	5.34	127.88	120.29
5	E	147	HIS	CA-C-N	5.34	127.75	120.54
5	E	147	HIS	C-N-CA	5.34	127.75	120.54
8	H	134	ASN	N-CA-C	5.34	118.09	110.24
1	A	602	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	1130	PHE	N-CA-C	-5.34	102.19	109.71
2	B	433	GLN	CA-C-N	5.33	127.96	120.28
2	B	433	GLN	C-N-CA	5.33	127.96	120.28
1	A	973	ILE	CB-CA-C	5.33	117.31	111.08
2	B	527	THR	CB-CA-C	5.33	117.17	109.45
2	B	1009	ASP	N-CA-C	-5.33	106.91	113.41
2	B	1013	ASN	N-CA-C	5.33	116.36	109.65
1	A	475	THR	CA-C-N	5.30	128.82	120.97
1	A	475	THR	C-N-CA	5.30	128.82	120.97
2	B	111	ALA	CA-C-N	5.30	129.68	121.26
2	B	111	ALA	C-N-CA	5.30	129.68	121.26
1	A	375	THR	CB-CA-C	5.29	119.83	109.35
2	B	945	GLU	CA-C-N	5.29	131.65	121.54
2	B	945	GLU	C-N-CA	5.29	131.65	121.54
4	D	52	LEU	CA-C-N	5.29	131.65	121.54
4	D	52	LEU	C-N-CA	5.29	131.65	121.54
5	E	118	PRO	CA-C-N	5.29	127.63	120.65
5	E	118	PRO	C-N-CA	5.29	127.63	120.65
5	E	60	PHE	N-CA-C	5.29	117.42	109.23
2	B	645	SER	N-CA-C	-5.28	105.60	111.36
1	A	438	ASP	CA-CB-CG	5.28	117.88	112.60
3	C	238	ILE	N-CA-CB	-5.28	105.99	111.64
8	H	145	ARG	CA-C-N	5.28	131.20	121.70
8	H	145	ARG	C-N-CA	5.28	131.20	121.70
2	B	320	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	804	TYR	CA-C-N	5.26	127.60	120.65
1	A	804	TYR	C-N-CA	5.26	127.60	120.65
2	B	359	GLU	N-CA-C	5.26	119.76	112.45
2	B	680	THR	CA-C-N	5.25	129.49	120.71
2	B	680	THR	C-N-CA	5.25	129.49	120.71
1	A	1393	ASN	N-CA-C	5.25	118.81	112.93
1	A	1266	THR	N-CA-C	-5.25	105.47	111.14
10	J	60	PHE	CA-CB-CG	5.25	119.05	113.80
2	B	621	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	670	ILE	N-CA-CB	5.25	116.98	111.00
1	A	939	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	1143	LEU	CA-C-N	5.24	127.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1143	LEU	C-N-CA	5.24	127.31	120.28
2	B	1176	ASN	N-CA-C	-5.24	106.73	113.23
2	B	318	VAL	N-CA-C	-5.24	105.43	110.72
5	E	160	GLU	CA-C-N	5.24	127.25	120.44
5	E	160	GLU	C-N-CA	5.24	127.25	120.44
9	I	8	ARG	N-CA-C	-5.24	101.89	109.59
10	J	14	VAL	CB-CA-C	5.24	116.69	110.93
1	A	884	ASP	CA-C-N	5.23	127.55	120.38
1	A	884	ASP	C-N-CA	5.23	127.55	120.38
2	B	642	ASP	CA-C-N	5.23	131.53	121.54
2	B	642	ASP	C-N-CA	5.23	131.53	121.54
2	B	472	ALA	CA-C-N	5.21	131.48	121.54
2	B	472	ALA	C-N-CA	5.21	131.48	121.54
3	C	78	GLU	CB-CG-CD	5.20	121.45	112.60
2	B	1121	GLY	CA-C-N	5.20	127.50	120.38
2	B	1121	GLY	C-N-CA	5.20	127.50	120.38
7	G	76	ALA	N-CA-C	5.20	116.71	108.96
3	C	172	PRO	CA-C-N	5.20	130.96	122.07
3	C	172	PRO	C-N-CA	5.20	130.96	122.07
1	A	898	ARG	N-CA-C	5.20	117.20	109.25
2	B	483	LEU	N-CA-C	5.19	118.09	110.30
8	H	104	PHE	CA-C-N	5.19	129.04	121.31
8	H	104	PHE	C-N-CA	5.19	129.04	121.31
11	K	62	LYS	N-CA-C	5.19	116.83	108.32
2	B	465	ASN	CA-CB-CG	5.18	117.78	112.60
6	F	72	LYS	CA-C-N	5.18	131.43	121.54
6	F	72	LYS	C-N-CA	5.18	131.43	121.54
7	G	32	GLU	N-CA-C	-5.17	105.72	111.36
2	B	222	ILE	N-CA-C	5.17	115.42	107.77
2	B	916	THR	CB-CA-C	5.17	115.67	109.31
1	A	718	VAL	CA-C-N	5.17	127.54	120.46
1	A	718	VAL	C-N-CA	5.17	127.54	120.46
1	A	1280	GLU	N-CA-C	5.15	116.98	108.48
1	A	871	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	757	ASN	CA-CB-CG	5.13	117.73	112.60
9	I	112	SER	N-CA-C	-5.13	105.91	113.61
3	C	42	PRO	CA-C-N	5.13	130.78	122.53
3	C	42	PRO	C-N-CA	5.13	130.78	122.53
1	A	478	TYR	CA-C-N	5.12	131.31	121.54
1	A	478	TYR	C-N-CA	5.12	131.31	121.54
1	A	922	ASP	CA-C-N	5.12	127.13	120.28
1	A	922	ASP	C-N-CA	5.12	127.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	60	ALA	N-CA-C	5.11	121.69	110.80
3	C	181	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	769	SER	N-CA-C	5.10	117.73	109.06
2	B	1181	GLU	N-CA-C	5.10	121.66	110.80
1	A	345	VAL	N-CA-C	5.09	116.69	108.85
2	B	56	ASP	N-CA-C	5.08	116.90	111.36
2	B	339	THR	CB-CA-C	5.08	120.29	109.10
9	I	94	ASP	CA-C-N	5.08	131.24	121.54
9	I	94	ASP	C-N-CA	5.08	131.24	121.54
1	A	35	ILE	CB-CA-C	5.07	121.75	111.60
5	E	100	ILE	CA-C-N	5.07	127.39	120.54
5	E	100	ILE	C-N-CA	5.07	127.39	120.54
1	A	1331	SER	CA-C-N	5.06	127.57	120.28
1	A	1331	SER	C-N-CA	5.06	127.57	120.28
11	K	85	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	256	GLN	CA-C-N	5.06	131.20	121.54
1	A	256	GLN	C-N-CA	5.06	131.20	121.54
8	H	59	ILE	CB-CA-C	5.06	119.58	111.29
2	B	882	THR	N-CA-C	-5.04	106.27	112.72
2	B	1070	GLU	CA-C-N	-5.03	116.08	122.37
2	B	1070	GLU	C-N-CA	-5.03	116.08	122.37
2	B	732	SER	N-CA-C	5.03	115.17	108.38
2	B	1180	PHE	CA-CB-CG	-5.03	108.77	113.80
9	I	119	THR	CB-CA-C	5.03	117.52	109.27
2	B	101	MET	N-CA-C	5.03	116.71	109.07
1	A	466	SER	N-CA-C	5.03	121.51	110.80
2	B	629	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	562	THR	CB-CA-C	5.03	117.51	109.62
2	B	726	ALA	N-CA-C	5.03	118.51	112.38
2	B	790	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	709	THR	N-CA-C	-5.02	104.24	110.41
1	A	1438	THR	N-CA-C	5.02	118.17	111.75
1	A	222	LEU	N-CA-C	-5.01	103.43	110.35
1	A	1198	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	234	MET	N-CA-C	-5.01	106.68	112.89
3	C	253	LYS	CA-C-N	5.01	127.24	120.38
3	C	253	LYS	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11197	0	11257	265	0
2	B	8859	0	8901	194	0
3	C	2095	0	2051	65	0
4	D	1434	0	1460	24	0
5	E	1752	0	1776	29	0
6	F	679	0	701	19	0
7	G	1340	0	1357	36	0
8	H	1068	0	1040	24	0
9	I	971	0	927	15	0
10	J	532	0	542	16	0
11	K	920	0	929	20	0
12	L	363	0	386	6	0
13	N	183	0	104	2	0
14	P	90	0	44	1	0
15	T	345	0	192	10	0
16	A	31	0	14	2	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	31868	0	31681	642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.41	1.02
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.47	0.96
3:C:46:ILE:HD12	3:C:46:ILE:H	1.38	0.87
2:B:1017:ILE:HD13	2:B:1017:ILE:H	1.41	0.86
10:J:48:ARG:O	10:J:52:THR:HG22	1.76	0.85
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.59	0.84
1:A:450:LEU:HD12	1:A:450:LEU:H	1.42	0.83
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.59	0.83
13:N:6:DA:H61	15:T:12:DT:H3	1.25	0.81
3:C:163:ILE:HD11	3:C:165:LYS:HB2	1.62	0.81
1:A:41:MET:HB2	1:A:49:LYS:HA	1.64	0.79
1:A:1193:LEU:HD21	1:A:1264:GLU:HB3	1.65	0.79
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.78
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.64	0.78
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.67	0.77
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.68	0.75
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.68	0.75
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.69	0.75
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.23	0.73
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.70	0.73
6:F:118:LEU:O	6:F:122:MET:HG3	1.88	0.73
3:C:46:ILE:H	3:C:46:ILE:CD1	2.03	0.72
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.71	0.71
15:T:16:DT:H2'	15:T:17:DT:H5''	1.72	0.71
1:A:679:ILE:HG13	1:A:732:LEU:HD12	1.73	0.70
8:H:4:THR:HA	8:H:60:ALA:HB2	1.73	0.70
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.75	0.69
1:A:40:THR:HG22	1:A:41:MET:HG3	1.74	0.69
7:G:1:MET:HE1	7:G:80:LYS:O	1.92	0.69
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.73	0.69
2:B:64:CYS:HA	2:B:67:SER:HB3	1.74	0.69
7:G:1:MET:CG	7:G:2:PHE:H	2.06	0.68
1:A:315:LEU:HA	1:A:321:PRO:HA	1.75	0.68
1:A:216:VAL:O	1:A:220:THR:HB	1.94	0.68
2:B:244:LEU:HD11	2:B:250:PHE:HD2	1.57	0.68
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.76	0.68
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.76	0.68
7:G:26:LEU:HB3	7:G:56:ILE:HD11	1.76	0.68
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.76	0.67
3:C:46:ILE:HD13	3:C:67:LEU:O	1.93	0.67
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.30	0.67
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LEU:O	1:A:633:VAL:HG23	1.94	0.66
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.77	0.66
10:J:8:PHE:H	10:J:49:MET:HE3	1.59	0.66
8:H:89:LEU:C	8:H:91:ASP:H	2.01	0.66
2:B:542:MET:HE2	2:B:747:MET:HG3	1.78	0.66
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.61	0.66
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.78	0.66
1:A:352:VAL:HB	2:B:1099:VAL:HG23	1.78	0.66
5:E:197:LYS:HG3	5:E:211:TYR:CE1	2.31	0.66
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.76	0.66
2:B:822:ASN:O	10:J:48:ARG:NH1	2.28	0.65
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.79	0.65
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.79	0.65
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.77	0.65
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.78	0.64
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.79	0.64
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.31	0.64
2:B:512:ARG:HD3	2:B:533:CYS:O	1.98	0.64
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.78	0.64
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.80	0.64
8:H:82:PRO:C	8:H:84:ALA:H	2.03	0.64
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.80	0.64
1:A:140:THR:HA	1:A:143:LYS:HD3	1.80	0.64
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.98	0.63
1:A:567:LYS:HA	1:A:568:PRO:C	2.23	0.63
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.33	0.63
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.64	0.63
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.14	0.63
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.81	0.62
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.62
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.64	0.62
7:G:34:VAL:O	7:G:37:SER:HB3	1.99	0.62
11:K:21:ILE:HG23	11:K:33:ILE:CG1	2.28	0.62
1:A:873:MET:HG3	1:A:1056:SER:O	2.00	0.62
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.38	0.61
1:A:262:LEU:HD21	1:A:325:ILE:HG12	1.82	0.61
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.63	0.61
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.82	0.61
2:B:880:THR:HB	2:B:934:LYS:HD2	1.83	0.61
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.82	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:LEU:HD13	12:L:44:ASP:HB2	1.82	0.61
15:T:15:DT:H2'	15:T:16:DT:C6	2.35	0.60
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.83	0.60
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.83	0.60
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.83	0.60
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.32	0.60
1:A:827:THR:O	1:A:831:THR:HB	2.01	0.60
2:B:234:ILE:HG21	2:B:237:VAL:HG22	1.84	0.60
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.84	0.60
1:A:35:ILE:O	1:A:84:ILE:HG22	2.02	0.59
1:A:41:MET:CB	1:A:49:LYS:HA	2.31	0.59
1:A:227:VAL:HG12	4:D:15:LEU:HD23	1.83	0.59
2:B:291:ILE:HD12	2:B:291:ILE:H	1.67	0.59
4:D:5:THR:HG21	7:G:74:TYR:OH	2.01	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.84	0.59
4:D:54:GLU:O	4:D:58:VAL:HG23	2.03	0.59
5:E:3:GLN:HE21	5:E:5:ASN:HB2	1.67	0.59
7:G:13:LEU:HD22	7:G:17:PHE:HD2	1.68	0.59
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.83	0.59
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.85	0.59
1:A:986:ILE:O	1:A:990:VAL:HG23	2.04	0.58
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.68	0.58
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.84	0.58
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.85	0.58
1:A:499:ALA:HB2	6:F:118:LEU:HD11	1.85	0.58
1:A:1172:LEU:C	1:A:1174:PHE:H	2.11	0.58
1:A:98:LYS:O	1:A:102:VAL:HG23	2.04	0.58
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.86	0.58
7:G:129:SER:HB3	7:G:138:THR:HG23	1.85	0.58
1:A:709:THR:HB	1:A:712:GLU:H	1.69	0.57
3:C:56:THR:HG22	3:C:57:VAL:H	1.69	0.57
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.86	0.57
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.86	0.57
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.87	0.57
3:C:56:THR:HG22	3:C:57:VAL:HG22	1.86	0.57
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.39	0.57
7:G:1:MET:SD	7:G:2:PHE:N	2.74	0.57
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.70	0.57
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.87	0.57
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.25	0.57
1:A:923:LEU:HD12	1:A:923:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ALA:O	5:E:19:VAL:HG23	2.05	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.86	0.56
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.87	0.56
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.86	0.56
1:A:1451:VAL:HG13	7:G:20:PRO:HB3	1.86	0.56
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.87	0.56
10:J:57:ILE:O	10:J:60:PHE:HB2	2.05	0.56
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.40	0.56
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.86	0.56
1:A:448:PRO:O	1:A:449:SER:HB2	2.06	0.56
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.06	0.56
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.86	0.56
4:D:32:GLU:HG3	7:G:5:LYS:HZ1	1.70	0.56
1:A:175:ARG:HH12	1:A:199:LEU:HD21	1.69	0.56
2:B:128:LEU:HB3	2:B:167:ILE:HD12	1.88	0.56
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.88	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.87	0.56
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.19	0.55
1:A:1343:ALA:HB2	5:E:150:VAL:HG13	1.86	0.55
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.88	0.55
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.88	0.55
1:A:78:PRO:O	1:A:245:PRO:HG2	2.07	0.55
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.55
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.87	0.55
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.88	0.55
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.05	0.55
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.89	0.55
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.72	0.55
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.87	0.55
15:T:16:DT:H2'	15:T:17:DT:C5'	2.36	0.55
1:A:392:VAL:HG13	1:A:415:LEU:HD21	1.88	0.55
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.07	0.55
2:B:882:THR:HB	2:B:934:LYS:C	2.32	0.55
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.89	0.55
2:B:492:LEU:HB2	2:B:751:VAL:HG11	1.88	0.55
1:A:578:LEU:HD23	1:A:612:ILE:HD11	1.89	0.54
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.87	0.54
11:K:18:LYS:HE3	11:K:38:GLU:HG2	1.89	0.54
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.08	0.54
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.71	0.54
2:B:497:ARG:HH22	2:B:775:LYS:HD3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.32	0.54
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.89	0.54
2:B:174:LEU:HD11	2:B:204:ILE:HD12	1.90	0.54
1:A:851:HIS:HE1	1:A:857:ARG:HB2	1.73	0.54
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.90	0.54
8:H:13:SER:HB2	8:H:27:GLU:HB3	1.89	0.54
1:A:63:ARG:HG3	1:A:74:MET:HG3	1.90	0.54
2:B:1006:ILE:HG23	10:J:43:ARG:HD2	1.89	0.54
10:J:7:CYS:O	10:J:11:GLY:HA2	2.08	0.54
2:B:788:ARG:O	2:B:967:ARG:NH1	2.41	0.54
8:H:100:THR:HG23	8:H:138:GLU:HA	1.90	0.54
2:B:244:LEU:CD1	2:B:250:PHE:HD2	2.19	0.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.41	0.53
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.90	0.53
2:B:295:GLY:H	2:B:298:LEU:HD13	1.73	0.53
2:B:916:THR:HB	2:B:935:ARG:HG3	1.90	0.53
2:B:281:PRO:HD2	2:B:284:ILE:HD13	1.91	0.53
1:A:194:ALA:HA	1:A:195:ASP:C	2.34	0.53
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.43	0.53
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.90	0.53
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.90	0.53
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.39	0.53
10:J:24:LEU:HD21	10:J:38:ARG:HD2	1.91	0.53
3:C:183:TRP:HB2	3:C:185:LYS:HE2	1.90	0.53
15:T:16:DT:C2'	15:T:17:DT:H5''	2.38	0.53
3:C:124:LEU:O	3:C:127:ARG:HG2	2.08	0.53
15:T:13:DA:H4'	15:T:14:DC:OP1	2.09	0.53
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.90	0.53
13:N:6:DA:N6	15:T:12:DT:H3	2.02	0.53
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.72	0.52
1:A:981:LEU:HD23	1:A:1039:LYS:HD2	1.89	0.52
2:B:425:THR:HA	2:B:428:ILE:HD12	1.91	0.52
1:A:35:ILE:HG22	1:A:270:LEU:HD21	1.91	0.52
1:A:153:PRO:HA	1:A:161:LEU:HA	1.91	0.52
2:B:654:ARG:H	2:B:657:HIS:CE1	2.27	0.52
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.91	0.52
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.90	0.52
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.92	0.52
1:A:1025:ARG:HA	1:A:1030:ARG:HH11	1.75	0.52
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.92	0.52
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.73	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.91	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.25	0.52
1:A:885:THR:OG1	1:A:1024:SER:HB2	2.09	0.52
2:B:310:MET:HE2	2:B:386:LEU:HB2	1.91	0.52
2:B:497:ARG:NH2	2:B:775:LYS:HD3	2.25	0.52
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.91	0.52
3:C:62:PHE:O	3:C:66:ARG:HG3	2.09	0.52
2:B:711:GLU:CB	2:B:712:PRO:HD3	2.40	0.51
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.36	0.51
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.09	0.51
1:A:637:LYS:HB3	1:A:641:VAL:CG1	2.41	0.51
5:E:97:VAL:HG13	5:E:127:ILE:HG12	1.91	0.51
1:A:335:ARG:HH12	2:B:1114:LEU:HD21	1.75	0.51
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.40	0.51
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.74	0.51
2:B:865:LYS:HD2	2:B:961:LEU:HD21	1.93	0.51
6:F:111:LEU:HD12	6:F:111:LEU:H	1.74	0.51
1:A:942:PHE:O	1:A:945:GLU:HB2	2.10	0.51
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.91	0.51
1:A:937:VAL:O	1:A:941:LYS:HG2	2.11	0.51
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.92	0.51
1:A:62:ASP:C	1:A:64:ASN:H	2.17	0.51
1:A:743:VAL:O	1:A:747:VAL:HG23	2.11	0.51
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.46	0.51
3:C:125:MET:SD	3:C:125:MET:N	2.84	0.51
4:D:27:LEU:HD23	4:D:197:SER:HB3	1.92	0.51
8:H:103:LYS:HB3	8:H:115:TYR:HD2	1.76	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.76	0.50
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.93	0.50
6:F:79:ARG:NH2	6:F:150:GLU:OE2	2.44	0.50
9:I:103:CYS:HB3	9:I:107:SER:H	1.76	0.50
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.92	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.51	0.50
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.92	0.50
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.93	0.50
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.93	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.94	0.50
2:B:509:ALA:O	2:B:511:PRO:HD3	2.11	0.50
2:B:542:MET:HG2	2:B:747:MET:HB3	1.92	0.50
3:C:20:PHE:HE2	3:C:22:LEU:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.94	0.50
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.94	0.50
1:A:1341:ILE:HD12	1:A:1376:THR:HG23	1.94	0.50
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.12	0.50
2:B:852:ARG:HG2	2:B:973:ILE:HG13	1.92	0.50
1:A:873:MET:C	1:A:1058:VAL:HG22	2.37	0.50
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.50
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.50
1:A:62:ASP:HB3	1:A:65:LEU:HB2	1.94	0.49
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.93	0.49
1:A:542:GLU:O	1:A:546:VAL:HG23	2.12	0.49
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.93	0.49
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.93	0.49
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.77	0.49
2:B:882:THR:C	2:B:884:ARG:H	2.20	0.49
4:D:8:PHE:HB2	4:D:38:ILE:HD12	1.94	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.94	0.49
1:A:1329:THR:HG23	1:A:1335:ILE:HG12	1.94	0.49
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.94	0.49
1:A:332:LYS:H	1:A:337:ARG:HB2	1.78	0.49
1:A:738:LYS:HD3	1:A:740:LEU:HD21	1.94	0.49
2:B:806:THR:HG22	2:B:808:ALA:H	1.77	0.49
3:C:146:LYS:HD2	10:J:57:ILE:HG12	1.95	0.49
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.76	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	0.49
1:A:373:THR:HG21	2:B:1105:ALA:CB	2.41	0.49
1:A:472:LEU:O	1:A:475:THR:HG22	2.12	0.49
1:A:927:VAL:O	1:A:931:GLU:HB2	2.13	0.49
2:B:1017:ILE:H	2:B:1017:ILE:CD1	2.10	0.49
4:D:127:ASP:HA	4:D:130:LEU:HD12	1.94	0.49
7:G:106:MET:HG2	7:G:107:LYS:N	2.26	0.49
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.27	0.49
4:D:126:ILE:HG21	4:D:145:MET:HB3	1.95	0.49
7:G:1:MET:CG	7:G:2:PHE:N	2.75	0.49
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.93	0.49
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.94	0.49
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.49
2:B:613:VAL:HG22	2:B:628:THR:HA	1.94	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.95	0.49
11:K:12:LEU:HD22	11:K:16:GLU:HB3	1.95	0.49
1:A:940:ARG:O	1:A:944:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.78	0.49
3:C:163:ILE:HD12	3:C:165:LYS:H	1.76	0.49
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.95	0.48
2:B:62:ILE:HG12	2:B:418:LYS:HD3	1.94	0.48
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.95	0.48
2:B:270:LYS:NZ	2:B:281:PRO:HG3	2.27	0.48
2:B:848:ARG:HH12	2:B:996:ARG:HD3	1.78	0.48
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.28	0.48
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.95	0.48
7:G:49:LEU:HD11	7:G:77:VAL:HG23	1.94	0.48
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.93	0.48
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.48
1:A:1163:ILE:HD13	1:A:1194:ARG:HD2	1.95	0.48
2:B:280:ILE:HB	2:B:285:ILE:HD11	1.94	0.48
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.39	0.48
1:A:440:ASP:O	1:A:460:VAL:HG23	2.13	0.48
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.95	0.48
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.95	0.48
2:B:908:GLU:HG3	2:B:943:SER:HA	1.96	0.48
3:C:40:GLU:HA	3:C:163:ILE:HD13	1.95	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:HD2	1.96	0.48
3:C:164:ALA:HA	3:C:167:HIS:O	2.14	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.78	0.48
1:A:492:PRO:CB	1:A:497:THR:HG22	2.43	0.48
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.48
2:B:638:PHE:HB3	2:B:651:LEU:HD23	1.96	0.48
3:C:146:LYS:HB2	10:J:57:ILE:HD11	1.94	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.44	0.48
6:F:106:PRO:HG2	7:G:18:PHE:C	2.38	0.48
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.39	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.48
2:B:343:ILE:O	2:B:344:LYS:HB2	2.11	0.48
11:K:87:LEU:O	11:K:91:CYS:HB2	2.14	0.47
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.96	0.47
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.96	0.47
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.96	0.47
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.48	0.47
7:G:19:GLY:O	7:G:22:MET:HB2	2.14	0.47
8:H:82:PRO:C	8:H:84:ALA:N	2.72	0.47
1:A:534:LEU:O	1:A:574:GLY:HA3	2.14	0.47
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:VAL:O	5:E:23:VAL:HG23	2.13	0.47
7:G:96:GLN:H	7:G:96:GLN:HG3	1.48	0.47
1:A:344:ARG:HG2	2:B:1127:GLY:O	2.14	0.47
2:B:758:PHE:HE1	2:B:1050:ILE:HD13	1.79	0.47
1:A:448:PRO:CG	16:A:2455:APC:H2	2.45	0.47
2:B:567:GLU:H	2:B:567:GLU:HG2	1.44	0.47
2:B:796:LEU:HD12	2:B:852:ARG:O	2.13	0.47
5:E:20:LYS:HD3	5:E:35:VAL:HA	1.97	0.47
1:A:246:VAL:O	1:A:328:ARG:NH1	2.39	0.47
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.96	0.47
6:F:147:SER:H	6:F:150:GLU:HG2	1.78	0.47
1:A:270:LEU:HD12	1:A:274:ILE:HD11	1.97	0.47
1:A:518:LYS:HE2	1:A:624:SER:O	2.15	0.47
1:A:711:ARG:HG2	9:I:97:MET:HE2	1.95	0.47
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.47
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.95	0.47
3:C:55:THR:HB	3:C:152:GLU:H	1.80	0.47
8:H:89:LEU:O	8:H:91:ASP:N	2.47	0.47
11:K:45:LEU:HD21	11:K:94:ILE:HG21	1.96	0.47
15:T:21:DC:H2'	15:T:22:BRU:H6	1.95	0.47
1:A:535:THR:HG22	1:A:575:LYS:HA	1.97	0.47
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.14	0.47
3:C:250:THR:HA	3:C:253:LYS:HD2	1.96	0.47
4:D:189:ASP:O	4:D:193:THR:HB	2.15	0.47
1:A:50:ILE:C	1:A:52:GLY:H	2.22	0.47
1:A:1451:VAL:O	1:A:1454:MET:HE2	2.14	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.96	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.97	0.47
1:A:352:VAL:HG12	1:A:467:THR:HG22	1.98	0.46
1:A:1025:ARG:O	1:A:1035:TYR:HE2	1.98	0.46
2:B:780:VAL:HB	2:B:817:LEU:HD23	1.97	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.46
3:C:256:ALA:HA	3:C:259:LEU:HD23	1.97	0.46
1:A:806:ARG:HH21	2:B:729:ILE:HG13	1.80	0.46
2:B:487:THR:HG23	2:B:490:SER:H	1.80	0.46
9:I:6:PHE:HB3	9:I:11:ASN:O	2.16	0.46
2:B:341:LEU:HD12	2:B:343:ILE:H	1.79	0.46
1:A:12:ARG:HB3	2:B:1218:THR:HG21	1.97	0.46
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.98	0.46
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.81	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.98	0.46
3:C:169:LYS:HE3	3:C:170:TRP:CH2	2.50	0.46
1:A:1142:THR:HG22	1:A:1271:ILE:O	2.16	0.46
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.97	0.46
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.81	0.46
2:B:126:SER:CB	2:B:172:ILE:HD11	2.46	0.46
3:C:125:MET:HE3	3:C:125:MET:HA	1.97	0.46
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.96	0.46
11:K:20:LYS:HB3	11:K:34:THR:HB	1.97	0.46
1:A:255:SER:HB2	2:B:918:ILE:HD11	1.96	0.46
1:A:671:ALA:H	1:A:676:MET:HE2	1.81	0.46
1:A:869:GLY:O	5:E:204:THR:HG21	2.15	0.46
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.50	0.46
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.97	0.46
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.98	0.46
2:B:542:MET:HE3	2:B:743:ILE:HD13	1.98	0.46
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.98	0.46
3:C:56:THR:HG21	3:C:145:CYS:SG	2.55	0.46
7:G:62:LEU:HD11	7:G:69:GLU:HB2	1.98	0.46
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.98	0.45
1:A:528:LEU:HD21	1:A:619:LYS:HG3	1.98	0.45
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.97	0.45
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.45
2:B:664:THR:HG23	2:B:678:GLU:N	2.31	0.45
3:C:244:VAL:O	3:C:248:ILE:HG13	2.16	0.45
4:D:176:GLU:OE2	4:D:201:LYS:HE2	2.15	0.45
6:F:82:THR:HG22	6:F:84:TYR:HB2	1.98	0.45
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.96	0.45
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.81	0.45
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.99	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.97	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.98	0.45
2:B:641:GLU:HB3	2:B:643:ASP:CG	2.42	0.45
2:B:1133:MET:O	2:B:1136:ASP:HB2	2.17	0.45
2:B:101:MET:HE3	2:B:169:ARG:NH2	2.31	0.45
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.99	0.45
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.47	0.45
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.98	0.45
1:A:70:CYS:O	1:A:70:CYS:SG	2.74	0.45
1:A:744:LYS:O	1:A:748:MET:HG3	2.17	0.45
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:LEU:HD22	9:I:48:LEU:HD21	1.98	0.45
2:B:54:PHE:HA	2:B:58:THR:HB	1.98	0.45
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.82	0.45
1:A:448:PRO:HG3	16:A:2455:APC:H2	1.98	0.45
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.99	0.45
2:B:839:MET:CE	2:B:980:PHE:HB2	2.47	0.45
3:C:52:GLU:HA	12:L:64:LEU:HD21	1.99	0.45
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.99	0.45
2:B:210:LYS:HD3	2:B:482:VAL:HG13	1.99	0.44
2:B:314:LEU:O	2:B:318:VAL:HG23	2.17	0.44
2:B:627:PHE:HB3	2:B:629:ASP:HB2	1.98	0.44
3:C:100:THR:CG2	3:C:119:VAL:HG13	2.47	0.44
9:I:82:GLU:HG2	9:I:104:LEU:HD13	1.98	0.44
1:A:484:GLY:H	2:B:989:THR:HG23	1.83	0.44
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.98	0.44
3:C:184:ASN:HD21	3:C:189:THR:H	1.63	0.44
1:A:1400:CYS:C	1:A:1402:PHE:H	2.26	0.44
3:C:172:PRO:O	3:C:235:VAL:HG23	2.17	0.44
7:G:99:PHE:CD1	7:G:115:MET:HE2	2.53	0.44
8:H:103:LYS:HB3	8:H:115:TYR:CD2	2.52	0.44
1:A:851:HIS:CE1	1:A:857:ARG:HB2	2.53	0.44
1:A:928:LEU:HB3	1:A:987:VAL:HG11	2.00	0.44
1:A:1006:ILE:HD13	5:E:164:LEU:HA	1.98	0.44
3:C:70:ILE:HG12	3:C:142:VAL:HG11	2.00	0.44
4:D:187:THR:C	4:D:189:ASP:N	2.74	0.44
6:F:153:VAL:HG12	6:F:155:LEU:HD12	1.99	0.44
12:L:31:CYS:HA	12:L:56:LEU:HD23	1.99	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	2.00	0.44
2:B:1083:ALA:HA	2:B:1084:GLN:HE21	1.82	0.44
7:G:112:LYS:HE2	7:G:120:THR:HG22	1.99	0.44
1:A:18:GLN:NE2	1:A:1418:LEU:HD12	2.32	0.44
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.98	0.44
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.99	0.44
5:E:17:ARG:HA	5:E:20:LYS:HD2	1.99	0.44
5:E:124:VAL:O	5:E:132:ILE:HD12	2.18	0.44
1:A:332:LYS:H	1:A:337:ARG:CB	2.31	0.44
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	2.00	0.44
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.99	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.61	0.44
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.51	0.44
4:D:27:LEU:HD23	4:D:197:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:C	1:A:56:PRO:HB3	2.42	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD12	2.00	0.44
2:B:509:ALA:C	2:B:511:PRO:HD3	2.43	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.99	0.44
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.44
9:I:4:PHE:HE2	9:I:13:MET:HB2	1.83	0.44
1:A:383:TYR:O	1:A:384:ASN:HB3	2.17	0.43
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.86	0.43
2:B:424:LEU:HD22	2:B:453:ILE:HD11	2.00	0.43
2:B:658:ILE:HG23	2:B:662:MET:HE2	1.99	0.43
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.18	0.43
1:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
1:A:883:LEU:HD13	1:A:943:LEU:HD22	2.00	0.43
2:B:776:GLN:HA	2:B:1096:ARG:HD3	2.00	0.43
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.43
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.00	0.43
8:H:109:LYS:HD3	8:H:111:LEU:HB2	2.00	0.43
1:A:1444:MET:HG3	7:G:60:ARG:HA	2.00	0.43
2:B:209:GLU:CD	2:B:788:ARG:HH22	2.26	0.43
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.99	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.39	0.43
2:B:1016:ALA:HB3	2:B:1017:ILE:HD13	2.01	0.43
1:A:265:LYS:O	1:A:269:ILE:HG13	2.18	0.43
2:B:69:LEU:HB2	2:B:90:ILE:HG22	1.99	0.43
2:B:666:TYR:C	2:B:668:ASP:H	2.27	0.43
3:C:96:SER:HB2	3:C:158:VAL:HG12	2.00	0.43
5:E:116:ILE:HB	5:E:121:MET:HE2	1.99	0.43
6:F:82:THR:HG22	6:F:84:TYR:H	1.83	0.43
1:A:418:SER:O	1:A:420:ARG:N	2.52	0.43
1:A:922:ASP:HB3	1:A:925:LEU:HD12	2.00	0.43
3:C:240:VAL:O	3:C:244:VAL:HG23	2.18	0.43
7:G:132:SER:HB3	7:G:135:ASP:H	1.83	0.43
1:A:84:ILE:HG13	1:A:239:LEU:HB3	2.00	0.43
1:A:747:VAL:HG21	1:A:758:ILE:HD12	2.01	0.43
1:A:945:GLU:HB3	5:E:201:LYS:HE3	1.99	0.43
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.43	0.43
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.99	0.43
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.49	0.43
1:A:140:THR:O	1:A:143:LYS:HG2	2.18	0.43
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.34	0.43
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.82	0.43
2:B:227:LYS:HG3	2:B:395:GLN:HG3	1.99	0.43
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.01	0.43
2:B:1017:ILE:HG12	2:B:1018:PRO:HD3	2.01	0.43
3:C:4:GLU:HB3	3:C:5:GLY:H	1.57	0.43
3:C:149:LYS:C	3:C:151:GLN:H	2.26	0.43
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.00	0.43
1:A:450:LEU:H	1:A:450:LEU:CD1	2.13	0.43
1:A:673:GLY:N	1:A:674:PRO:HD2	2.33	0.43
1:A:1406:VAL:HG12	1:A:1410:PHE:CE2	2.54	0.43
4:D:135:GLY:C	4:D:137:ASN:H	2.27	0.43
5:E:135:PHE:HB3	5:E:140:LEU:HD11	2.01	0.43
1:A:105:CYS:SG	1:A:139:TRP:HA	2.59	0.43
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.54	0.43
1:A:381:THR:HG22	1:A:384:ASN:CG	2.43	0.43
1:A:639:PRO:HD2	1:A:640:GLN:H	1.83	0.43
2:B:67:SER:HB2	2:B:92:PHE:HD2	1.84	0.43
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.33	0.43
1:A:135:PHE:HE1	1:A:222:LEU:HD23	1.84	0.42
1:A:325:ILE:HD12	2:B:1210:MET:HG3	1.99	0.42
2:B:705:MET:HE3	2:B:705:MET:HA	2.01	0.42
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.58	0.42
5:E:5:ASN:HA	5:E:8:ASN:ND2	2.34	0.42
1:A:418:SER:C	1:A:420:ARG:H	2.27	0.42
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.49	0.42
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.01	0.42
2:B:114:PRO:HG3	2:B:181:LEU:HD11	2.01	0.42
2:B:291:ILE:HG22	2:B:297:ILE:HG13	2.01	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:HB2	2.01	0.42
1:A:531:ILE:HD13	1:A:622:VAL:HG21	2.00	0.42
1:A:586:ILE:HD11	1:A:633:VAL:HA	2.01	0.42
1:A:672:ASP:HB3	1:A:674:PRO:HD2	2.00	0.42
1:A:818:MET:HA	2:B:514:LEU:HB3	2.02	0.42
1:A:1059:HIS:O	1:A:1060:PRO:C	2.60	0.42
1:A:1116:LEU:HD12	1:A:1311:VAL:HA	2.01	0.42
2:B:365:THR:HG21	2:B:370:PHE:CG	2.55	0.42
3:C:38:ILE:HG13	3:C:176:ILE:HD12	2.01	0.42
1:A:453:MET:O	1:A:456:MET:HE2	2.19	0.42
1:A:701:LEU:H	1:A:701:LEU:HG	1.56	0.42
2:B:294:ASP:HB2	9:I:13:MET:H	1.84	0.42
2:B:453:ILE:HD12	2:B:453:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:HG12	2:B:991:GLY:O	2.19	0.42
7:G:62:LEU:HA	7:G:63:PRO:HD2	1.82	0.42
8:H:24:CYS:HB2	8:H:44:VAL:HG21	2.01	0.42
1:A:662:PHE:HB3	2:B:829:CYS:HB2	2.00	0.42
1:A:1111:MET:H	1:A:1111:MET:HG2	1.66	0.42
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.54	0.42
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.83	0.42
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.01	0.42
2:B:797:TYR:HB2	2:B:852:ARG:O	2.20	0.42
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.86	0.42
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.85	0.42
6:F:76:LYS:O	6:F:79:ARG:NH1	2.48	0.42
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.77	0.42
1:A:1006:ILE:HB	5:E:167:ARG:HG3	2.00	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.85	0.42
2:B:1185:CYS:C	2:B:1187:ASN:H	2.28	0.42
3:C:101:LEU:HD22	3:C:155:LEU:HD12	2.01	0.42
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.02	0.42
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.67	0.42
15:T:16:DT:C2'	15:T:17:DT:C5'	2.97	0.42
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.85	0.42
3:C:50:GLU:HG3	12:L:66:GLN:HG3	2.00	0.42
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.85	0.42
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.20	0.42
1:A:646:PHE:O	1:A:650:GLN:HG2	2.20	0.42
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.54	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:CB	2.49	0.42
3:C:29:MET:HE2	11:K:94:ILE:HG23	2.01	0.42
1:A:926:GLN:O	1:A:930:ASP:HB2	2.20	0.42
8:H:84:ALA:HA	8:H:87:ARG:HD2	2.00	0.42
1:A:354:SER:O	1:A:469:ARG:HA	2.20	0.42
1:A:913:LEU:HD12	1:A:915:SER:OG	2.19	0.42
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.68	0.42
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.34	0.42
2:B:604:ARG:HG2	2:B:611:PRO:HA	2.02	0.42
2:B:1001:PHE:HB3	2:B:1007:VAL:HG23	2.02	0.42
7:G:153:GLN:HB3	7:G:156:SER:O	2.20	0.42
1:A:830:LYS:HD3	1:A:1098:VAL:HG21	2.02	0.41
2:B:193:LYS:HB3	2:B:787:VAL:HG21	2.02	0.41
2:B:522:VAL:HG12	2:B:539:LEU:HA	2.01	0.41
2:B:713:ALA:HA	2:B:733:HIS:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.36	0.41
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.49	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.03	0.41
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.02	0.41
2:B:184:ALA:HB1	2:B:188:ASP:HB2	2.02	0.41
2:B:314:LEU:HD21	2:B:386:LEU:HD11	2.03	0.41
1:A:601:LYS:HD3	1:A:603:ASN:HD21	1.85	0.41
3:C:83:SER:HA	3:C:95:CYS:HB2	2.01	0.41
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.35	0.41
3:C:56:THR:HG23	3:C:147:LEU:HD23	2.02	0.41
1:A:154:SER:C	1:A:156:ASP:H	2.28	0.41
1:A:185:TRP:CZ3	1:A:200:ARG:HG3	2.56	0.41
1:A:523:ILE:HG23	1:A:527:THR:HB	2.03	0.41
2:B:661:LEU:HD21	2:B:684:LEU:HD11	2.03	0.41
2:B:756:ILE:O	2:B:759:PRO:HD3	2.21	0.41
5:E:69:ILE:H	5:E:69:ILE:HG13	1.64	0.41
14:P:9:G:H1	15:T:20:DC:H42	1.68	0.41
1:A:606:LEU:HG	1:A:613:ILE:HD13	2.03	0.41
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.02	0.41
1:A:1340:GLY:O	1:A:1342:GLU:N	2.54	0.41
2:B:705:MET:HE2	2:B:745:PRO:HB3	2.03	0.41
1:A:408:ASP:C	1:A:410:GLY:H	2.28	0.41
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.86	0.41
2:B:662:MET:HA	2:B:665:GLU:HB2	2.02	0.41
3:C:142:VAL:HG21	10:J:5:VAL:HG13	2.03	0.41
4:D:164:ILE:HG23	4:D:168:LYS:HD2	2.03	0.41
1:A:35:ILE:HA	1:A:52:GLY:O	2.21	0.41
1:A:1143:LEU:O	1:A:1147:THR:OG1	2.38	0.41
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.03	0.41
2:B:521:LEU:HA	2:B:543:SER:OG	2.21	0.41
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.85	0.41
3:C:116:LYS:C	3:C:118:LEU:H	2.28	0.41
6:F:109:VAL:HG22	6:F:110:ASP:N	2.36	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.54	0.41
8:H:89:LEU:C	8:H:91:ASP:N	2.71	0.41
1:A:708:MET:HG2	1:A:712:GLU:HB3	2.03	0.41
2:B:102:VAL:HG23	2:B:110:HIS:HB3	2.03	0.41
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.55	0.41
3:C:239:PRO:HG2	3:C:242:GLN:HB2	2.03	0.41
7:G:99:PHE:CE1	7:G:115:MET:HE2	2.56	0.41
1:A:341:MET:HE3	1:A:341:MET:HB3	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:O	1:A:519:PRO:HA	2.21	0.40
1:A:565:ILE:O	1:A:570:PRO:HA	2.21	0.40
1:A:763:ALA:O	1:A:803:SER:HB3	2.21	0.40
1:A:873:MET:HE3	1:A:957:PRO:HG3	2.02	0.40
1:A:1148:ILE:HG23	9:I:49:ILE:HB	2.03	0.40
3:C:98:VAL:H	3:C:122:SER:HB3	1.84	0.40
7:G:145:VAL:HG22	7:G:163:ILE:CG2	2.51	0.40
2:B:603:LEU:HD12	2:B:609:ILE:HG13	2.02	0.40
10:J:58:GLU:HA	10:J:61:LEU:HD12	2.03	0.40
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.40
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	2.03	0.40
4:D:70:PHE:O	4:D:74:GLN:HB2	2.21	0.40
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.77	0.40
11:K:35:PHE:O	11:K:70:ARG:HA	2.21	0.40
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.04	0.40
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.03	0.40
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.03	0.40
2:B:806:THR:HB	2:B:809:MET:HG3	2.04	0.40
2:B:908:GLU:O	2:B:940:PRO:HB2	2.21	0.40
2:B:1048:THR:HB	2:B:1049:ASP:H	1.76	0.40
11:K:7:PHE:HB2	11:K:11:LEU:HD22	2.03	0.40
1:A:30:ILE:HA	2:B:1183:LYS:HE3	2.03	0.40
1:A:311:GLN:O	1:A:312:PRO:C	2.63	0.40
2:B:371:GLU:H	2:B:371:GLU:CD	2.30	0.40
7:G:111:THR:HB	7:G:114:LEU:HD23	2.03	0.40
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1417/1732 (82%)	1198 (84%)	145 (10%)	74 (5%)	1	17
2	B	1095/1224 (90%)	916 (84%)	127 (12%)	52 (5%)	2	19
3	C	264/318 (83%)	236 (89%)	20 (8%)	8 (3%)	3	26
4	D	174/221 (79%)	146 (84%)	19 (11%)	9 (5%)	1	17
5	E	212/215 (99%)	192 (91%)	15 (7%)	5 (2%)	4	29
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	10	41
7	G	169/171 (99%)	152 (90%)	14 (8%)	3 (2%)	6	34
8	H	129/146 (88%)	99 (77%)	19 (15%)	11 (8%)	0	10
9	I	117/122 (96%)	94 (80%)	20 (17%)	3 (3%)	4	28
10	J	63/70 (90%)	52 (82%)	5 (8%)	6 (10%)	0	8
11	K	113/120 (94%)	106 (94%)	7 (6%)	0	100	100
12	L	44/70 (63%)	21 (48%)	13 (30%)	10 (23%)	0	1
All	All	3879/4564 (85%)	3286 (85%)	411 (11%)	182 (5%)	2	19

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	69	THR
1	A	78	PRO
1	A	169	ASN
1	A	193	ASP
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	331	GLY
1	A	335	ARG
1	A	384	ASN
1	A	775	ILE
1	A	1206	ASP
1	A	1341	ILE
1	A	1405	THR
2	B	108	VAL
2	B	208	SER
2	B	229	ALA
2	B	282	ILE
2	B	340	ALA

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Mol	Chain	Res	Type
2	B	344	LYS
2	B	368	GLU
2	B	473	MET
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1107	ALA
4	D	16	LYS
4	D	18	VAL
6	F	73	ALA
7	G	2	PHE
7	G	63	PRO
7	G	154	VAL
8	H	90	ALA
9	I	9	ASP
10	J	6	ARG
12	L	28	LYS
12	L	45	ALA
12	L	50	ASP
1	A	41	MET
1	A	43	GLU
1	A	167	CYS
1	A	189	ARG
1	A	224	PHE
1	A	257	ARG
1	A	409	SER
1	A	419	LYS
1	A	449	SER
1	A	569	LYS
1	A	639	PRO
1	A	922	ASP
1	A	1124	HIS
1	A	1175	SER
1	A	1242	VAL
1	A	1255	GLU

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Mol	Chain	Res	Type
1	A	1365	TYR
1	A	1366	ARG
1	A	1394	THR
1	A	1401	SER
2	B	322	PHE
2	B	338	GLY
2	B	341	LEU
2	B	343	ILE
2	B	371	GLU
2	B	526	GLU
2	B	772	ALA
2	B	867	GLY
2	B	1096	ARG
2	B	1157	ALA
3	C	215	GLU
3	C	237	SER
4	D	27	LEU
4	D	53	SER
8	H	17	PRO
8	H	81	PRO
8	H	83	GLN
9	I	95	THR
10	J	13	VAL
10	J	57	ILE
12	L	39	SER
12	L	55	ILE
12	L	56	LEU
1	A	73	GLY
1	A	76	GLU
1	A	155	GLU
1	A	195	ASP
1	A	197	PRO
1	A	312	PRO
1	A	332	LYS
1	A	418	SER
1	A	421	ALA
1	A	465	TYR
1	A	916	GLY
1	A	1002	GLY
1	A	1403	GLU
2	B	531	GLN
2	B	648	HIS

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Mol	Chain	Res	Type
2	B	655	LYS
2	B	667	GLN
2	B	734	HIS
2	B	792	MET
2	B	831	SER
2	B	1155	SER
2	B	1156	ASP
2	B	1188	LYS
3	C	90	ASP
3	C	184	ASN
3	C	214	ASN
4	D	119	ARG
4	D	198	LEU
4	D	199	ASN
5	E	48	ASP
8	H	32	THR
8	H	78	SER
8	H	82	PRO
8	H	128	ASN
10	J	3	VAL
12	L	26	THR
12	L	59	ALA
1	A	187	LYS
1	A	448	PRO
1	A	466	SER
1	A	870	GLU
2	B	476	ARG
3	C	117	ASP
3	C	150	GLY
4	D	15	LEU
5	E	36	GLU
5	E	50	MET
8	H	19	ARG
8	H	60	ALA
8	H	89	LEU
10	J	64	ASN
12	L	53	HIS
1	A	35	ILE
1	A	62	ASP
1	A	196	GLU
1	A	567	LYS
1	A	599	SER

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	958	VAL
2	B	764	SER
2	B	1143	ALA
2	B	1221	SER
5	E	145	THR
5	E	174	GLN
9	I	47	GLU
10	J	2	ILE
12	L	38	LEU
1	A	117	GLU
1	A	479	ASN
1	A	672	ASP
1	A	1122	PRO
2	B	305	VAL
2	B	395	GLN
2	B	466	TRP
2	B	870	ILE
2	B	1181	GLU
4	D	218	GLU
1	A	178	GLY
1	A	283	GLY
2	B	907	GLY
1	A	61	ILE
2	B	436	VAL
2	B	743	ILE
3	C	38	ILE
1	A	51	GLY
1	A	244	PRO
1	A	310	GLY
2	B	364	ILE
1	A	385	ILE
1	A	1388	GLY
1	A	910	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1243/1519 (82%)	1001 (80%)	242 (20%)	1	9
2	B	966/1061 (91%)	782 (81%)	184 (19%)	1	10
3	C	234/274 (85%)	187 (80%)	47 (20%)	1	8
4	D	160/200 (80%)	123 (77%)	37 (23%)	1	5
5	E	196/197 (100%)	167 (85%)	29 (15%)	3	16
6	F	74/137 (54%)	61 (82%)	13 (18%)	2	12
7	G	152/152 (100%)	124 (82%)	28 (18%)	1	11
8	H	117/128 (91%)	98 (84%)	19 (16%)	2	14
9	I	113/116 (97%)	98 (87%)	15 (13%)	4	19
10	J	60/65 (92%)	47 (78%)	13 (22%)	1	6
11	K	99/102 (97%)	78 (79%)	21 (21%)	1	7
12	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3454/4008 (86%)	2792 (81%)	662 (19%)	1	9

All (662) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	22	PHE
1	A	23	SER
1	A	28	ARG
1	A	34	LYS
1	A	39	GLU
1	A	41	MET
1	A	42	ASP
1	A	43	GLU
1	A	44	THR
1	A	53	LEU
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	117	GLU
1	A	126	LEU
1	A	132	LYS

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Mol	Chain	Res	Type
1	A	143	LYS
1	A	144	THR
1	A	145	LYS
1	A	147	VAL
1	A	157	ASP
1	A	159	THR
1	A	164	ARG
1	A	174	ILE
1	A	175	ARG
1	A	188	ASP
1	A	195	ASP
1	A	204	THR
1	A	208	LEU
1	A	220	THR
1	A	226	GLU
1	A	227	VAL
1	A	232	GLU
1	A	236	LEU
1	A	237	THR
1	A	238	CYS
1	A	247	ARG
1	A	250	ILE
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	290	GLU
1	A	293	GLU
1	A	295	LEU
1	A	299	HIS
1	A	307	ASP
1	A	308	ILE
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG
1	A	344	ARG
1	A	352	VAL
1	A	369	SER
1	A	375	THR
1	A	378	GLU
1	A	383	TYR
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	386	ASP
1	A	391	LEU
1	A	393	ARG
1	A	398	GLU
1	A	403	LYS
1	A	406	ILE
1	A	408	ASP
1	A	423	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	438	ASP
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	455	MET
1	A	461	LYS
1	A	463	ILE
1	A	466	SER
1	A	470	LEU
1	A	472	LEU
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	493	GLN
1	A	497	THR
1	A	498	ARG
1	A	500	GLU
1	A	504	LEU
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	526	ASP
1	A	527	THR
1	A	536	LEU
1	A	538	ASP
1	A	545	GLN
1	A	549	MET
1	A	560	ILE

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Mol	Chain	Res	Type
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	584	ASN
1	A	588	LEU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	645	LEU
1	A	651	LYS
1	A	657	LEU
1	A	666	ILE
1	A	670	ILE
1	A	680	THR
1	A	685	GLU
1	A	691	LEU
1	A	701	LEU
1	A	711	ARG
1	A	719	VAL
1	A	734	GLU
1	A	738	LYS
1	A	756	ILE
1	A	758	ILE
1	A	768	GLN
1	A	770	VAL
1	A	773	LYS
1	A	775	ILE
1	A	783	THR
1	A	788	SER
1	A	791	ASP
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	842	VAL

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Mol	Chain	Res	Type
1	A	843	LYS
1	A	864	ILE
1	A	886	ILE
1	A	890	ASP
1	A	896	ARG
1	A	905	ASP
1	A	908	LEU
1	A	915	SER
1	A	919	ILE
1	A	926	GLN
1	A	927	VAL
1	A	930	ASP
1	A	948	VAL
1	A	960	ILE
1	A	973	ILE
1	A	976	THR
1	A	980	ASP
1	A	982	THR
1	A	987	VAL
1	A	993	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1005	GLU
1	A	1009	ASN
1	A	1016	THR
1	A	1024	SER
1	A	1036	ARG
1	A	1038	THR
1	A	1040	GLN
1	A	1052	GLN
1	A	1058	VAL
1	A	1064	VAL
1	A	1067	LEU
1	A	1080	THR
1	A	1096	SER
1	A	1098	VAL
1	A	1111	MET
1	A	1113	THR
1	A	1116	LEU
1	A	1124	HIS
1	A	1134	ILE
1	A	1135	ARG

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Mol	Chain	Res	Type
1	A	1142	THR
1	A	1145	SER
1	A	1146	VAL
1	A	1147	THR
1	A	1159	ARG
1	A	1170	ILE
1	A	1173	HIS
1	A	1176	LEU
1	A	1193	LEU
1	A	1195	LEU
1	A	1197	LEU
1	A	1208	THR
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1260	LEU
1	A	1274	ARG
1	A	1276	VAL
1	A	1283	VAL
1	A	1290	LYS
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1314	SER
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1335	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1356	ILE
1	A	1366	ARG
1	A	1381	LEU
1	A	1383	SER
1	A	1387	HIS
1	A	1391	ARG
1	A	1400	CYS
1	A	1403	GLU
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1425	SER
1	A	1426	GLU
1	A	1432	GLN
1	A	1436	ILE
1	A	1442	ASP
1	A	1443	VAL
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
1	A	1453	TYR
2	B	25	ILE
2	B	35	SER
2	B	44	VAL
2	B	46	GLN
2	B	56	ASP
2	B	63	ILE
2	B	91	SER
2	B	97	VAL
2	B	102	VAL
2	B	108	VAL
2	B	118	ARG
2	B	122	LEU
2	B	126	SER
2	B	128	LEU
2	B	130	VAL
2	B	167	ILE
2	B	169	ARG
2	B	170	LEU
2	B	199	MET
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	241	ARG
2	B	261	ARG
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	276	ILE
2	B	278	GLN
2	B	280	ILE
2	B	287	ARG
2	B	294	ASP

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Mol	Chain	Res	Type
2	B	305	VAL
2	B	324	ILE
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	361	LEU
2	B	365	THR
2	B	368	GLU
2	B	370	PHE
2	B	387	LEU
2	B	393	LYS
2	B	395	GLN
2	B	398	ARG
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	418	LYS
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	454	THR
2	B	469	GLN
2	B	481	GLN
2	B	482	VAL
2	B	485	ARG
2	B	489	SER
2	B	502	ILE
2	B	513	GLN
2	B	527	THR
2	B	529	GLU
2	B	531	GLN
2	B	544	CYS
2	B	545	ILE
2	B	547	VAL
2	B	552	MET
2	B	554	ILE
2	B	563	MET

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Mol	Chain	Res	Type
2	B	567	GLU
2	B	570	VAL
2	B	574	SER
2	B	576	ASP
2	B	580	VAL
2	B	595	ARG
2	B	602	THR
2	B	603	LEU
2	B	604	ARG
2	B	606	LYS
2	B	609	ILE
2	B	615	MET
2	B	616	ILE
2	B	619	ILE
2	B	620	ARG
2	B	628	THR
2	B	653	VAL
2	B	657	HIS
2	B	658	ILE
2	B	678	GLU
2	B	680	THR
2	B	685	LEU
2	B	689	LEU
2	B	691	GLU
2	B	708	GLU
2	B	723	VAL
2	B	731	VAL
2	B	736	THR
2	B	737	THR
2	B	743	ILE
2	B	754	SER
2	B	766	ARG
2	B	775	LYS
2	B	776	GLN
2	B	780	VAL
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	792	MET
2	B	815	ARG
2	B	816	GLU
2	B	824	ILE

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Mol	Chain	Res	Type
2	B	839	MET
2	B	844	SER
2	B	854	LEU
2	B	871	THR
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	885	MET
2	B	889	THR
2	B	891	ASP
2	B	895	ASP
2	B	899	ILE
2	B	906	SER
2	B	908	GLU
2	B	909	ASP
2	B	910	VAL
2	B	934	LYS
2	B	935	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	956	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	997	GLU
2	B	1002	THR
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1017	ILE
2	B	1026	LEU
2	B	1045	SER
2	B	1049	ASP
2	B	1050	ILE
2	B	1058	LEU
2	B	1060	ARG
2	B	1065	GLN

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Mol	Chain	Res	Type
2	B	1071	VAL
2	B	1072	MET
2	B	1084	GLN
2	B	1098	MET
2	B	1112	GLN
2	B	1113	VAL
2	B	1123	SER
2	B	1133	MET
2	B	1134	GLU
2	B	1137	CYS
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1149	GLU
2	B	1155	SER
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1175	LEU
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1203	LEU
2	B	1212	ILE
3	C	8	VAL
3	C	21	ILE
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	43	THR
3	C	46	ILE
3	C	52	GLU
3	C	53	THR
3	C	56	THR
3	C	58	LEU
3	C	78	GLU
3	C	81	GLU

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Mol	Chain	Res	Type
3	C	84	ARG
3	C	89	GLU
3	C	108	GLU
3	C	111	THR
3	C	119	VAL
3	C	121	VAL
3	C	122	SER
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	138	GLU
3	C	142	VAL
3	C	145	CYS
3	C	158	VAL
3	C	163	ILE
3	C	179	GLU
3	C	186	LEU
3	C	197	SER
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	248	ILE
3	C	260	LEU
3	C	262	LEU
3	C	263	THR
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	18	VAL
4	D	19	GLU
4	D	23	ASN
4	D	27	LEU
4	D	32	GLU
4	D	37	GLN

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Mol	Chain	Res	Type
4	D	38	ILE
4	D	43	GLU
4	D	46	GLU
4	D	47	LEU
4	D	64	VAL
4	D	65	GLU
4	D	67	ARG
4	D	76	LYS
4	D	123	LEU
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	156	ASP
4	D	159	THR
4	D	173	HIS
4	D	177	VAL
4	D	183	LEU
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	200	ASN
4	D	206	GLU
4	D	208	GLU
4	D	213	GLU
4	D	221	TYR
5	E	3	GLN
5	E	9	ILE
5	E	30	ILE
5	E	31	THR
5	E	40	GLU
5	E	41	ASP
5	E	46	TYR
5	E	60	PHE
5	E	65	THR
5	E	67	GLU
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	95	THR
5	E	107	THR

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Mol	Chain	Res	Type
5	E	126	SER
5	E	144	ILE
5	E	150	VAL
5	E	154	ILE
5	E	175	LEU
5	E	184	VAL
5	E	188	LEU
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	197	LYS
5	E	202	SER
6	F	72	LYS
6	F	77	ASP
6	F	78	GLN
6	F	97	ARG
6	F	110	ASP
6	F	111	LEU
6	F	118	LEU
6	F	119	ARG
6	F	123	LYS
6	F	129	LYS
6	F	152	ILE
6	F	153	VAL
6	F	155	LEU
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	31	LEU
7	G	34	VAL
7	G	37	SER
7	G	39	THR
7	G	55	ASP
7	G	64	THR
7	G	65	ASP
7	G	75	ARG
7	G	77	VAL
7	G	80	LYS
7	G	96	GLN
7	G	106	MET

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Mol	Chain	Res	Type
7	G	110	VAL
7	G	118	ASP
7	G	120	THR
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	141	SER
7	G	143	ILE
7	G	152	SER
7	G	155	SER
7	G	160	ILE
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	39	THR
8	H	49	VAL
8	H	54	SER
8	H	56	THR
8	H	76	THR
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	109	LYS
8	H	111	LEU
8	H	112	ILE
8	H	123	MET
8	H	130	ARG
8	H	144	ILE
9	I	8	ARG
9	I	26	LEU
9	I	31	THR
9	I	42	LEU
9	I	43	VAL
9	I	50	THR
9	I	51	ASN
9	I	52	ILE
9	I	59	VAL
9	I	94	ASP
9	I	104	LEU

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Mol	Chain	Res	Type
9	I	109	ILE
9	I	114	GLN
9	I	116	ASN
9	I	118	ARG
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	19	GLU
10	J	24	LEU
10	J	26	GLN
10	J	41	LEU
10	J	48	ARG
10	J	51	LEU
10	J	56	LEU
10	J	57	ILE
10	J	62	ARG
11	K	1	MET
11	K	5	ASP
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	21	ILE
11	K	25	THR
11	K	33	ILE
11	K	35	PHE
11	K	37	LYS
11	K	47	ARG
11	K	51	LEU
11	K	75	ILE
11	K	79	GLU
11	K	91	CYS
11	K	95	ILE
11	K	101	LEU
11	K	102	LYS
11	K	103	THR
11	K	108	GLU
11	K	114	LEU
12	L	27	LEU
12	L	28	LYS
12	L	33	GLU
12	L	38	LEU

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Mol	Chain	Res	Type
12	L	44	ASP
12	L	54	ARG
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	61	THR
12	L	63	ARG
12	L	64	LEU
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	GLN
1	A	160	GLN
1	A	169	ASN
1	A	209	ASN
1	A	339	ASN
1	A	451	HIS
1	A	490	HIS
1	A	587	HIS
1	A	626	ASN
1	A	640	GLN
1	A	698	GLN
1	A	760	GLN
1	A	811	GLN
1	A	851	HIS
1	A	965	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1070	GLN
1	A	1187	GLN
1	A	1232	ASN
1	A	1378	GLN
1	A	1390	ASN
2	B	46	GLN
2	B	47	GLN
2	B	115	GLN
2	B	300	HIS
2	B	306	ASN

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Mol	Chain	Res	Type
2	B	357	GLN
2	B	363	HIS
2	B	400	HIS
2	B	433	GLN
2	B	449	ASN
2	B	469	GLN
2	B	513	GLN
2	B	538	ASN
2	B	667	GLN
2	B	986	GLN
2	B	1062	HIS
2	B	1195	HIS
3	C	7	GLN
3	C	17	ASN
3	C	102	GLN
3	C	123	ASN
3	C	140	ASN
3	C	151	GLN
3	C	231	ASN
4	D	132	GLN
4	D	143	ASN
4	D	150	ASN
4	D	165	GLN
4	D	216	ASN
5	E	3	GLN
5	E	5	ASN
5	E	8	ASN
5	E	174	GLN
5	E	179	GLN
8	H	35	GLN
8	H	43	ASN
8	H	52	GLN
8	H	137	GLN
9	I	46	HIS
9	I	60	GLN
9	I	89	GLN
9	I	116	ASN
11	K	29	ASN
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/4 (75%)	2 (66%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G
14	P	10	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	BRU	T	22	14,15	18,21,22	0.80	0	25,30,33	2.33	10 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	14,15	-	4/7/21/22	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	5.20	119.32	113.34
15	T	22	BRU	O4-C4-C5	-4.70	119.80	125.80
15	T	22	BRU	C4-N3-C2	-4.07	122.00	127.34
15	T	22	BRU	N3-C2-N1	3.66	119.66	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C1'-N1-C2	3.52	124.55	117.66
15	T	22	BRU	O2-C2-N3	-3.32	115.36	121.49
15	T	22	BRU	C6-C5-C4	-2.75	117.88	120.67
15	T	22	BRU	C1'-N1-C6	-2.65	116.29	120.74
15	T	22	BRU	BR-C5-C4	2.45	120.85	118.02
15	T	22	BRU	C6-N1-C2	-2.15	119.17	121.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	O4'-C4'-C5'-O5'
15	T	22	BRU	C3'-C4'-C5'-O5'
15	T	22	BRU	C2'-C1'-N1-C2
15	T	22	BRU	C2'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	22	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	APC	A	2455	-	29,33,33	2.02	11 (37%)	44,52,52	1.95	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	APC	A	2455	-	-	1/19/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2455	APC	PB-O3B	4.90	1.63	1.58
16	A	2455	APC	PA-O1A	3.94	1.60	1.51
16	A	2455	APC	PG-O1G	3.84	1.62	1.50
16	A	2455	APC	PA-O2A	-3.59	1.47	1.56
16	A	2455	APC	C5-C4	2.94	1.44	1.39
16	A	2455	APC	C5-N7	-2.35	1.34	1.39
16	A	2455	APC	C6-N6	2.30	1.40	1.34
16	A	2455	APC	PB-O2B	2.27	1.61	1.56
16	A	2455	APC	O4'-C1'	2.24	1.47	1.42
16	A	2455	APC	C5'-C4'	2.16	1.58	1.51
16	A	2455	APC	PG-O2G	2.00	1.62	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2455	APC	C5-C4-N3	-5.58	119.04	126.72
16	A	2455	APC	PB-O3B-PG	-5.09	114.20	132.45
16	A	2455	APC	N3-C4-N9	4.51	134.83	127.17
16	A	2455	APC	C5-N7-C8	3.89	109.56	103.45
16	A	2455	APC	C4-C5-N7	-3.75	106.29	110.58
16	A	2455	APC	C2-N3-C4	2.96	119.06	111.83
16	A	2455	APC	N3-C2-N1	-2.44	124.89	128.58
16	A	2455	APC	O5'-C5'-C4'	2.22	116.55	108.99
16	A	2455	APC	O2G-PG-O3B	2.07	111.57	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

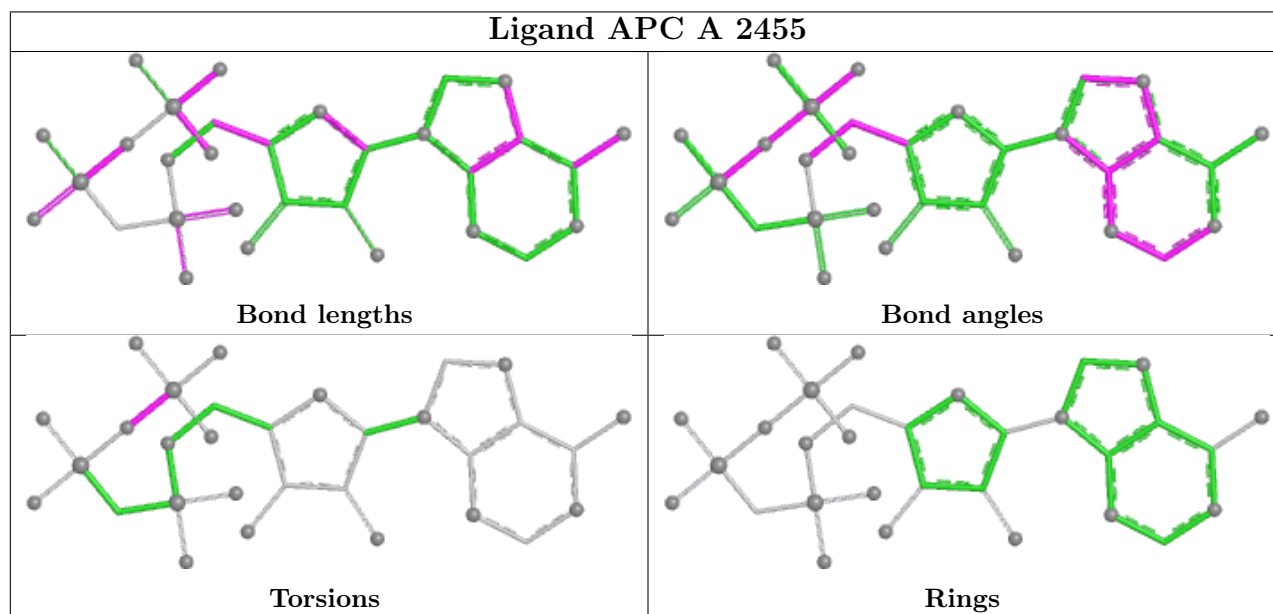
Mol	Chain	Res	Type	Atoms
16	A	2455	APC	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2455	APC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.72
1	B	351:TYR	C	352:ALA	N	3.12

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1425/1732 (82%)	-0.08	26 (1%) 67 47	84, 142, 199, 264	0
2	B	1115/1224 (91%)	0.07	24 (2%) 62 44	87, 157, 218, 237	0
3	C	266/318 (83%)	-0.19	1 (0%) 88 74	107, 144, 187, 216	0
4	D	178/221 (80%)	0.17	6 (3%) 48 34	115, 158, 205, 225	0
5	E	214/215 (99%)	-0.00	3 (1%) 73 52	116, 177, 224, 236	0
6	F	84/155 (54%)	-0.26	1 (1%) 76 55	85, 121, 151, 168	0
7	G	171/171 (100%)	-0.02	0 100 100	111, 139, 176, 198	0
8	H	133/146 (91%)	0.37	9 (6%) 23 21	151, 186, 222, 233	0
9	I	119/122 (97%)	0.12	4 (3%) 48 34	144, 192, 223, 236	0
10	J	65/70 (92%)	0.03	1 (1%) 72 50	119, 137, 182, 189	0
11	K	115/120 (95%)	-0.09	1 (0%) 81 62	112, 138, 180, 193	0
12	L	46/70 (65%)	0.65	5 (10%) 10 13	143, 208, 222, 231	0
13	N	9/14 (64%)	1.47	2 (22%) 2 4	271, 282, 299, 300	0
14	P	4/4 (100%)	0.94	0 100 100	208, 215, 222, 235	0
15	T	16/26 (61%)	1.01	1 (6%) 26 22	200, 241, 295, 296	0
All	All	3960/4608 (85%)	0.01	84 (2%) 63 44	84, 151, 215, 300	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1083	THR	8.0
2	B	509	ALA	5.5
12	L	25	ALA	4.6
2	B	446	LEU	4.4
8	H	63	LEU	4.4
1	A	1176	LEU	4.3
6	F	72	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1243	VAL	4.0
2	B	134	LYS	3.9
1	A	310	GLY	3.8
1	A	251	SER	3.8
1	A	190	ALA	3.6
2	B	251	ILE	3.6
12	L	62	LYS	3.5
1	A	1093	LYS	3.5
1	A	186	LYS	3.4
1	A	1082	ASN	3.3
2	B	708	GLU	3.2
1	A	3	GLY	3.1
13	N	10	DG	3.1
4	D	3	VAL	3.1
2	B	502	ILE	3.1
8	H	139	ASN	2.9
2	B	108	VAL	2.9
1	A	1081	LEU	2.8
5	E	91	LYS	2.8
11	K	114	LEU	2.8
1	A	309	ALA	2.8
1	A	880	LYS	2.8
9	I	3	THR	2.8
2	B	250	PHE	2.7
2	B	573	GLN	2.7
4	D	10	THR	2.7
2	B	341	LEU	2.7
4	D	187	THR	2.7
13	N	2	DA	2.7
8	H	132	LEU	2.7
2	B	262	GLU	2.6
2	B	263	GLY	2.6
2	B	70	ILE	2.6
2	B	345	LYS	2.6
2	B	709	ASP	2.6
15	T	24	DG	2.6
1	A	830	LYS	2.5
5	E	110	PHE	2.5
2	B	20	ASP	2.4
8	H	2	SER	2.4
2	B	584	GLY	2.4
12	L	26	THR	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	81	PRO	2.4
8	H	119	GLY	2.4
1	A	1080	THR	2.4
1	A	36	ARG	2.4
4	D	24	ALA	2.4
1	A	51	GLY	2.4
1	A	1321	GLY	2.4
1	A	252	PHE	2.3
2	B	1224	PHE	2.3
12	L	27	LEU	2.3
9	I	2	THR	2.3
2	B	726	ALA	2.3
8	H	84	ALA	2.3
1	A	1455	PRO	2.3
2	B	343	ILE	2.2
10	J	42	LYS	2.2
1	A	924	LYS	2.2
1	A	38	PRO	2.2
2	B	436	VAL	2.1
8	H	46	LEU	2.1
1	A	1362	TYR	2.1
1	A	176	LYS	2.1
1	A	1079	MET	2.1
12	L	53	HIS	2.0
3	C	268	ASP	2.0
9	I	52	ILE	2.0
1	A	1187	GLN	2.0
2	B	305	VAL	2.0
4	D	221	TYR	2.0
4	D	22	GLU	2.0
9	I	4	PHE	2.0
5	E	93	MET	2.0
8	H	77	ARG	2.0
2	B	243	ALA	2.0
2	B	1173	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	BRU	T	22	20/21	0.94	0.09	222,232,237,237	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

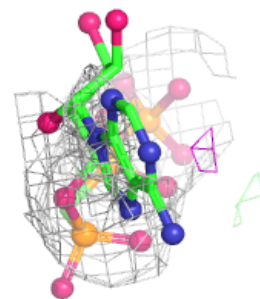
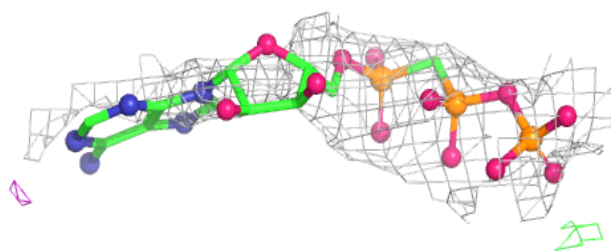
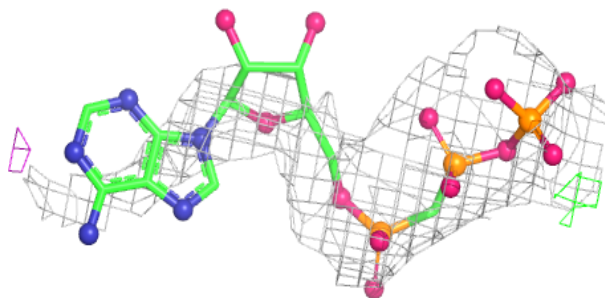
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	APC	A	2455	31/31	0.86	0.15	265,268,278,278	0
18	MG	A	2458	1/1	0.93	0.13	230,230,230,230	0
17	ZN	L	1071	1/1	0.99	0.04	235,235,235,235	0
17	ZN	I	1122	1/1	0.99	0.04	248,248,248,248	0
17	ZN	C	1269	1/1	1.00	0.05	129,129,129,129	0
17	ZN	I	1121	1/1	1.00	0.05	155,155,155,155	0
17	ZN	A	2456	1/1	1.00	0.03	177,177,177,177	0
17	ZN	J	1066	1/1	1.00	0.06	124,124,124,124	0
17	ZN	A	2457	1/1	1.00	0.03	101,101,101,101	0
17	ZN	B	2225	1/1	1.00	0.04	112,112,112,112	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around APC A 2455:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.